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SUPPORTING INFORMATION

Synthesis of 6-membered cyclic carbonates from 1,3-diols and low CO₂ pressure : a novel mild strategy to replace phosgene reagents

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1. Experimental Details

1.1 Materials and Methods

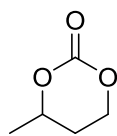
All manipulations were performed under atmosphere of argon or carbon dioxide using standard Schlenk techniques. Triethylamine (Aldrich) was refluxed and then distilled over CaH_2 prior to use. 1,2-*O*-Isopropylidene- α -D-xylofuranose (**1h**) was purchased from Carbosynth and used without further purification. All other reagents were purchased from either Sigma Aldrich or Alfa Aesar and used without further purification. All solvents used were dry and obtained *via* SPS (solvent purification system) except for anhydrous chloroform (containing amylenes as stabiliser) which was purchased from Sigma Aldrich. N4.5 CP grade CO_2 was purchased from BOC. Column chromatography was performed on silica gel and spots visualised with KMnO_4 solution. ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded on a Bruker 400 MHz instrument and referenced to residual solvent peaks. Coupling constants are given in Hertz. CHN microanalysis was performed by Mr Stephen Boyer of London Metropolitan University. Polarimetry measurements were made on an Optical Activity LTD AA-10 automatic polarimeter. $[\alpha]_{\text{D}}$ values are given in $10^{-1} \text{ deg cm}^2 \text{ g}^{-1}$.

1.2 General Procedure

Under an Argon atmosphere, a 1.7 M solution of diol (0.5 ml, 1 equiv.) in anhydrous chloroform was prepared. On a Schlenk line fed with CO_2 , the argon atmosphere was replaced with CO_2 by three cycles of vacuum followed by CO_2 . After allowing 10 minutes for the solution to become saturated with CO_2 , DBU (1 equiv.) was added dropwise (over a period of 1 hour) at room temperature with stirring and monitoring of the CO_2 uptake. After two hours stirring at room temperature no further CO_2 uptake was observed and triethylamine (1 equiv.) was added dropwise to the viscous solution. A solution of TsCl (0.5 M, 1 eq.) in anhydrous chloroform was then added dropwise and the reaction mixture left to stir overnight. Following removal of the solvent under reduced pressure, the cyclic carbonate product was isolated by column chromatography (5% acetone/ CHCl_3). All R_f values are reported for a 1:1 acetone: CHCl_3 eluent.

1.3 Characterisation of Cyclic Carbonates

4-Methyl-[1,3]-dioxan-2-one (2a)



Colourless oil (0.440 g, 68%); R_f 0.61. Found: C, 51.63; H, 7.04. $C_5H_8O_3$ requires C, 51.72; H 6.94%. δ_H (400 MHz, $CDCl_3$) 4.68-4.44 (1 H, m, CHMe), 4.46-4.21 (2 H, m, OCH_2), 2.06-2.00 (1 H, m, OCH_2CHH), 1.78-1.88 (1 H, m, OCH_2CHH), 1.35 (3 H, d, $J = 6.3$, CH_3); δ_C (101 MHz, $CDCl_3$) 148.9 (C=O), 75.7 (CH), 66.9 (CH_2O), 28.4 (CH_2), 20.9 (CH_3) in accordance with the literature.¹ HR-MS (ESI) [$C_5H_8O_3 + Na$]⁺ Theo. 139.0371 found 139.0386.

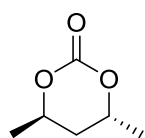
(R)-4-Methyl-[1,3]-dioxan-2-one (2a)

White crystalline solid (0.440 g, 68%). $[\alpha]_D^{25} +26$ (c 1.0 in $CHCl_3$).

(S)-4-Methyl-[1,3]-dioxan-2-one (2a)

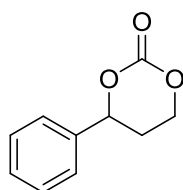
White crystalline solid (0.455 g, 70%). $[\alpha]_D^{25} -27$ (c 1.0 in $CHCl_3$).

4R,6R-Dimethyl-[1,3]-dioxan-2-one (2b)



Yellow oil (0.331 g, 53%); R_f 0.60. Found: C, 55.49; H, 7.61. $C_6H_{10}O_3$ requires C, 55.37; H, 7.75%. δ_H (400 MHz, $CDCl_3$) 4.74-4.66 (1 H, m, CHMe), 1.93 (1 H, t, $J = 5.6$, CHMe), 1.43 (3 H, d, $J = 6.5$, CH_3); δ_C (101 MHz, $CDCl_3$) 149.5 (C=O), 72.6 (CH), 34.0 (CH_2), 20.9 (CH_3) in accordance with the literature.¹⁻² HR-MS (ESI) [$C_6H_{10}O_3 + Na$]⁺ Theo. 153.0522 found 153.0556.

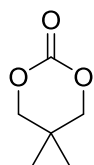
4-Phenyl-[1,3]-dioxan-2-one (2c)



1-Phenylpropane-1,3-diol (**1c**) was synthesised in two steps from acetophenone and dimethyl carbonate following the literature procedures.³ The cyclic carbonate was obtained as a colourless oil, which solidified other time (0.332 g, 55%); R_f 0.72. Found: C, 67.45; H, 5.74. $C_{10}H_{10}O_3$ requires C, 67.41; H, 5.66%. 1H NMR and ^{13}C NMR were consistent with previous reports.⁴ δ_H (400 MHz, $CDCl_3$) 7.48-7.32 (5 H, m, Ph-H), 5.52 (1 H, dd, $J = 9.8, 3.7$, CHO), 4.61-4.40 (2 H, m, CH_2O), 2.39-2.32 (1 H, m, OCH_2CHH), 2.30-2.20 (1 H, m, OCH_2CHH); δ_C (101 MHz, $CDCl_3$) 148.8 (C=O), 137.9 (quaternary C), 129.1 (*m*-PhC), 129.0 (*o*-PhC), 125.7 (*p*-PhC), 80.2 (CH), 66.9

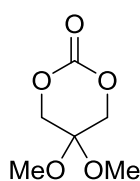
(CH₂O), 29.4 (CH₂). HR-MS (ESI) [C₁₀H₁₀O₃ + Na]⁺ Theo. 201.0528 found 201.0526.

5,5-Dimethyl-[1,3]-dioxolan-2-one (2d)



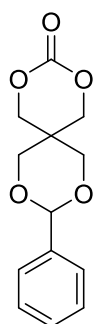
White powder (0.332 g, 53%); R_f 0.65. Found: C, 55.38; H, 7.67. C₆H₁₀O₃ requires C, 55.37; H, 7.75%. δ_{H} (400 MHz, CDCl₃) 4.04 (1 H, s, CH₂), 1.09 (2 H, s, CH₃); δ_{C} (101 MHz, CDCl₃) 148.2 (C=O), 77.5 (quaternary C), 28.5 (CH₂), 21.1 (CH₃) in accordance with the literature.⁵ HR-MS (ESI) [C₆H₁₀O₃ + Na]⁺ Theo. 131.0708 found. 131.0716.

5,5-Dimethoxy-[1,3]-dioxolan-2-one (2e)



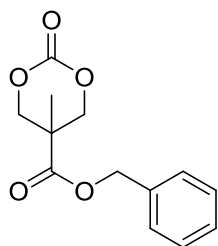
2,2-dimethoxy-propane-1,3-diol (**1e**) was prepared according to the literature procedure.⁶ The corresponding cyclic carbonate was obtained as a white powder (0.291 g, 49%); R_f 0.63. Found: C, 44.52; H, 6.35. C₆H₁₀O₅ requires C, 44.45; H, 6.22%. δ_{H} (400 MHz, CDCl₃) 4.28 (2 H, s, CH₂), 3.31 (3 H, s, CH₃); δ_{C} (101 MHz, CDCl₃) 147.9 (C=O), 92.2 (C), 69.9 (CH₂), 49.4 (OCH₃) in accordance with literature.⁵ HR-MS (ESI) [C₆H₁₀O₅ + Na]⁺ Theo. 185.0425 found 185.0434.

9-phenyl-2,4,8,10-tetraoxaspiro[5,5]undecanone (2f)



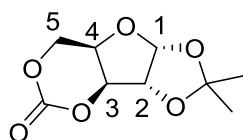
The benzylidene acetal-protected pentaerythritol diol (**1f**) was synthesised as previously reported in the literature.⁷ The corresponding cyclic carbonate was obtained as a white powder (0.257 g, 46%); R_f 0.62. Found: C, 62.23; H, 5.67. C₁₃H₁₄O₅ requires C, 62.39; H, 5.64%. δ_{H} (400 MHz, CDCl₃) 7.57-7.28 (5 H, m, Ph-H), 5.50 (1 H, s, CHPh), 4.70 (2 H, s, CH₂), 4.21 (2 H, dd, *J* = 10.6, 1.4, CH₂), 4.09 (2 H, s, CH₂), 3.88 (2 H, dd, *J* = 10.6, 1.4, CH₂); δ_{C} (101 MHz, CDCl₃) 148.0 (C=O), 137.0 (C), 129.5 (CH), 128.5 (CH), 126.0 (CH), 102.4 (CH), 71.4 (CH₂), 70.4 (CH₂), 69.4 (2 CH₂) in accordance with the literature.⁷ HR-MS (ESI) [C₁₃H₁₄O₅ + Na]⁺ Theo. 273.0738 found 273.0727.

Benzyl 5-methyl-2-oxo-1,3-dioxane-5-carboxylate (2g)



Benzyl protected bis-MPA (**1g**) was prepared according to the literature procedure.^{5, 8} The cyclic carbonate was isolated as a colourless oil, which crystallised on standing (0.229 g, 41%); R_f 0.66. Found: C, 62.25; H, 5.68. $C_{13}H_{14}O_5$ requires C, 62.39; H, 5.64%. δ_H 7.49-7.22 (5 H, m, Ar-H), 5.21 (2 H, s, CH₂), 4.70 (2 H, d, J = 10.9, CH₂), 4.20 (2 H, d, J = 10.9, CH₂), 1.32 (3 H, s, CH₃); δ_C (101 MHz, CDCl₃) 171.0 (C=O), 147.5 (C=O), 134.9 (ArC), 130.0 (ArC), 128.9 (ArC), 128.3 (ArC), 73.0 (2OCH₂), 68.0 (OCH₂Ph), 40.3 (C), 17.6 (CH₃) corresponding with the literature data.⁹ HR-MS (ESI) [$C_{13}H_{14}O_5$]⁺ Theo. 251.0914 found 251.0938.

Cyclic 1,2-*O*-isopropylidene-3,5-*O*-carbonate- α -D-xylofuranose (**2h**)



White powder (62.5 mg, 11%); R_f 0.51. Found: C, 49.98; H, 5.66. $C_9H_{12}O_6$ requires C, 50.00; H, 5.60%. δ_H (400 MHz, CDCl₃) 4.60 (1 H, d, J 3.7, H-1), 4.88 (1 H, d, J 2.8, H-3), 4.74 (1 H, d, J 3.7, H-2), 4.63-4.59 (1H, m, H-5a), 4.56-4.52 (2 H, m, H-4, H-5b), 1.50 (3 H, s, C(CH₃)₂), 1.33 (3 H, s, C(CH₃)₂); δ_C (101 MHz, CDCl₃) 146.4 (C=O), 113.1 (C(CH₃)₂), 105.3 (C-1), 83.9 (C-2), 82.5 (C-3), 69.2 (C-4), 66.8 (C-5), 26.8 (C(CH₃)₂), 26.3 (C(CH₃)₂) in agreement with the literature.¹⁰ HR-MS (ESI) [$C_9H_{12}O_6 + Na$]⁺ Theo. 239.0526 found 239.0592.

2. Assignment of CO₂ Insertion Products

In the case of all diols, CO₂ insertion was monitored by ¹H and ¹³C NMR and assignment of the mono- and bis- inserted products aided by COSY, HSQC and DEPT135 experiments. Assignment is shown for the reaction with 1,3-butanediol.

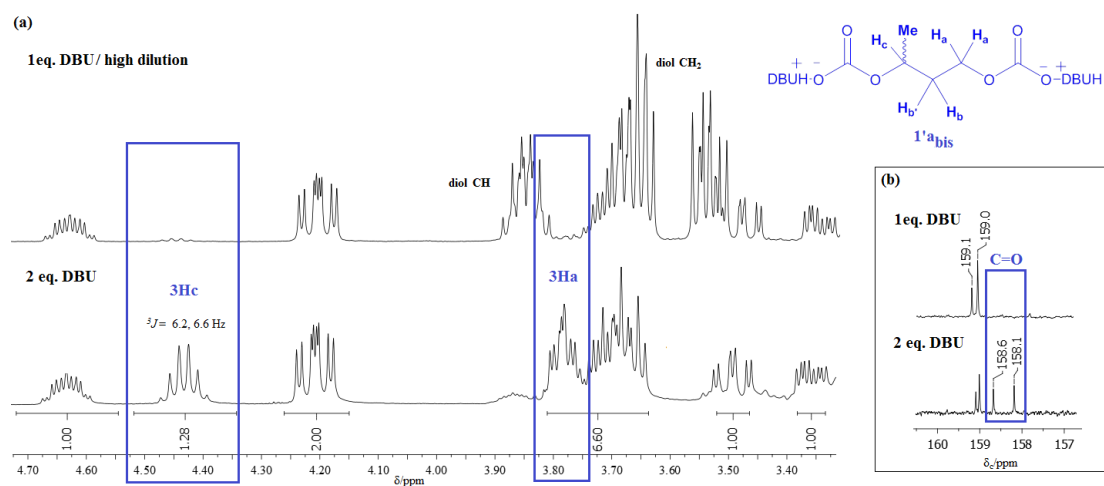


Figure S1: Assignment of **1'a_{bis}** showing (a) the ^1H NMR spectrum (400 MHz, CDCl_3) from 4.7 to 3.3 ppm of the reaction mixture with 1 equiv. (top) and to confirm assigned with 2 equiv. (bottom) of DBU (b) The ^{13}C NMR (101 MHz, CDCl_3) in the region assigned to the C=O resonances.

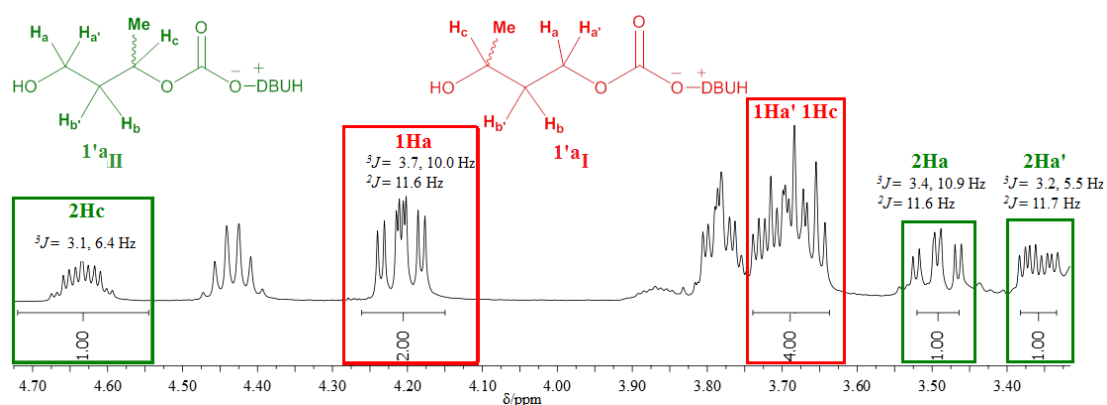


Figure S2: ^1H NMR (400 MHz, CDCl_3) showing assignments of H_a , $\text{H}_{a'}$ and H_c for mono-inserted products **1'a_I** and **1'a_{II}** based on COSY and HSQC experiments.

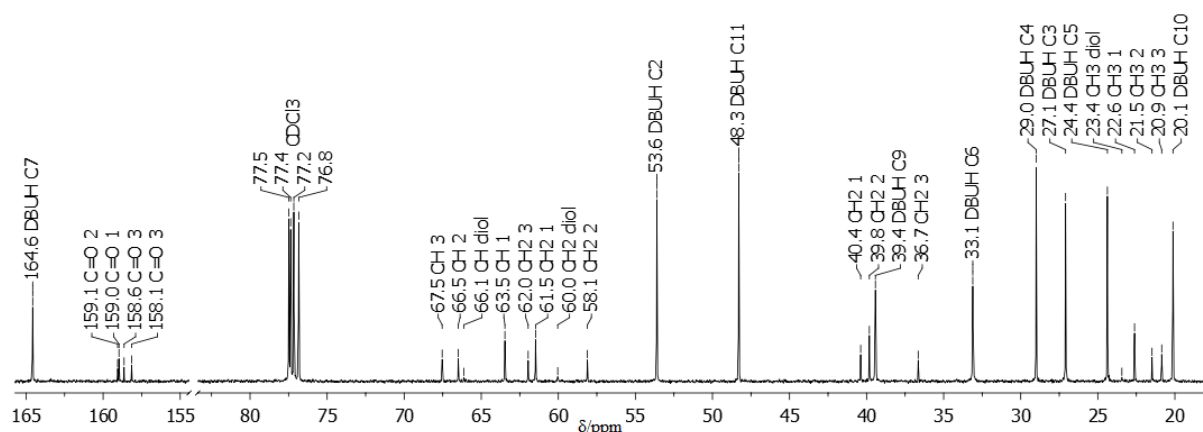


Figure S3: ^{13}C NMR (101 MHz, CDCl_3) following CO_2 insertion into **1a** with DBU.

3. DFT Computational Details

All calculations were performed using the Gaussian09 suite of codes (revision A.02).¹¹ Geometries were fully optimised without any symmetry or geometry constraints. The nature of all the stationary points as minima was verified by calculations of the vibrational frequency spectrum, and characterised by no imaginary mode. All transition states were characterized by precisely one imaginary mode corresponding to the intended reaction. Free energies were calculated within the harmonic approximation for vibrational frequencies.

Optimisation was carried out using the $\text{r}\omega\text{b97xD}$ LC hybrid functional developed by Chai and Head-Gordon that includes an empirical dispersion correction and has been shown to effectively reproduce thermodynamic and kinetic experimental data.¹² The 6-31+g(d) basis set was used at a temperature of 298K and solvent effects in chloroform considered using conductor-like polarisable continuum model (CPCM).

3.1 DFT Calculations for DBU-aided CO₂ Insertion and Ring-Closing

The low barrier for CO₂ insertion into the hydroxyl group via a ternary DBU, CO₂ diol mechanism is shown, as well as the high barrier for subsequent ring-closing in the absence of a leaving group strategy.

<i>Structure</i>	<i>G (Hartree)</i>	<i>ΔG (kcal mol⁻¹)</i>
DBU	-461.767329	-
CO ₂	-188.538882	-
(R)-1,3-butanediol	-308.698783	-
H ₂ O	-76.403072	-
Cyclic carbonate (CC)	-420.829745	-
Diol (+DBU+CO ₂)	-959.004994	0 (reference)
A	-958.99408	6.8
TS _{AB}	-958.983371	13.6
B	-959.014418	-5.9
TS _{BC}	-959.013594	-5.4
C	-959.018545	-8.5
D	-959.013651	-5.4
TS _{DE}	-958.946382	36.8
E	-958.970665	21.5
TS _{EF}	-958.961071	27.6
F	-958.98709	11.2
A'	-958.987274	11.1
TS _{AB'}	-958.974844	18.9
B'	-959.008702	-2.3
TS _{BC'}	-959.005974	-0.6
C'	-959.010334	-3.4
D'	-959.012944	-5.0
TS _{DE'}	-958.946125	36.9
E'	-958.969966	22.0
TS _{EF'}	-958.961087	27.6
F'	-958.990060	9.4
D S _N 2	-959.009702	-3.0
TS _{DE S_N2}	-958.921093	52.6
E S _N 2	-958.950345	34.3
[DBU-CO ₂] [‡] (+diol)	-958.988882	10.1
DBU-CO ₂ (+diol)	-959.001693	2.1
[DBU-CO ₂ --primary OH] [‡]	-958.932993	45.5
[DBU-CO ₂ --secondary OH] [‡]	-958.931713	46.0
Secondary OH-DBU adduct (+CO ₂)	-959.005540	-0.3
Primary OH-DBU adduct (+CO ₂)	-959.006135	-0.7
CC (+H ₂ O+DBU)	-959.000146	3.0

Table S1: Computed Free Gibbs Energies at the rob97xd/6-31+g(d)/cpcm=methanol/298K level of theory.

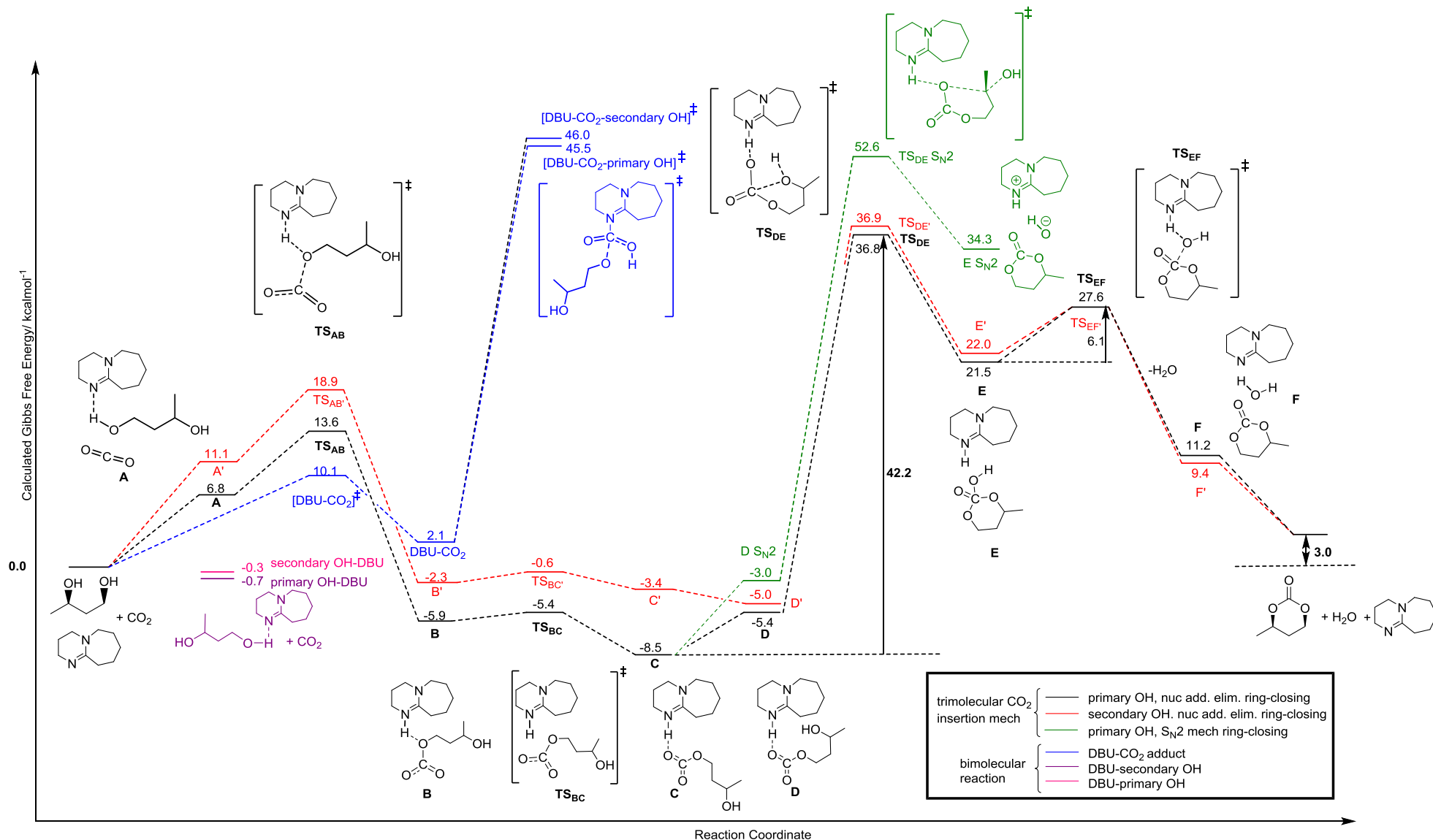


Figure S4: Calculated potential energy surface diagram at the 6-31+G(d)/r0b97xD/cpcm=MeOH/298K level for the reaction between DBU, CO₂ and (R)-1,3-butanediol. The scheme in black shows the trimolecular reaction at the primary hydroxyl group and in red at the secondary. Formation of the DBU-CO₂ adduct prior to reaction with either of the OH groups¹³ is shown in blue and interaction of the DBU with the primary or secondary OH groups prior to CO₂ insertion in purple and pink, respectively.

3.2 DFT Calculations for Tosylation and Subsequent Ring-Closing Steps

All combinations of ion pairs were computed but only the lowest in energy are reported.

<i>Structure</i>	<i>G (Hartree)</i>	<i>ΔG (kcal.mol⁻¹)</i>
NEt ₃	-292.161443	-
TsCl	-1279.492029	-
HNEt ₃ Cl	-752.986040	-
DBUHCl	-922.601085	-
Cyclic carbonate (CC)	-420.829745	-
I (+TsCl+ NEt ₃)	-2530.662493	0 (reference)
II	-2530.641749	13.0
III	-2530.615106	29.7
IV (+HNEt ₃ Cl)	-2238.487149	-25.4
V (+HNEt ₃ Cl)	-2238.538384	-3.1
VI (+HNEt ₃ Cl)	-2530.715343	-33.2
CC + DBUHOTs + HNEt ₃ Cl	-2530.721027	-36.7
VII	-2530.640391	13.9
VIII	-2530.624530	23.8
IX (+DBUHCl)	-2530.666091	-2.3
X (+DBUHCl)	-2530.636103	16.6
XI (+DBUHCl)	-2530.711971	-31.0
CC +NEt ₃ OTs + DBUHCl	-2530.714752	-32.8

Table S2: Computed Gibbs Free Energies at the rōb97xd/6-31+g(d)/cpcm=chloroform/298K level of theory.

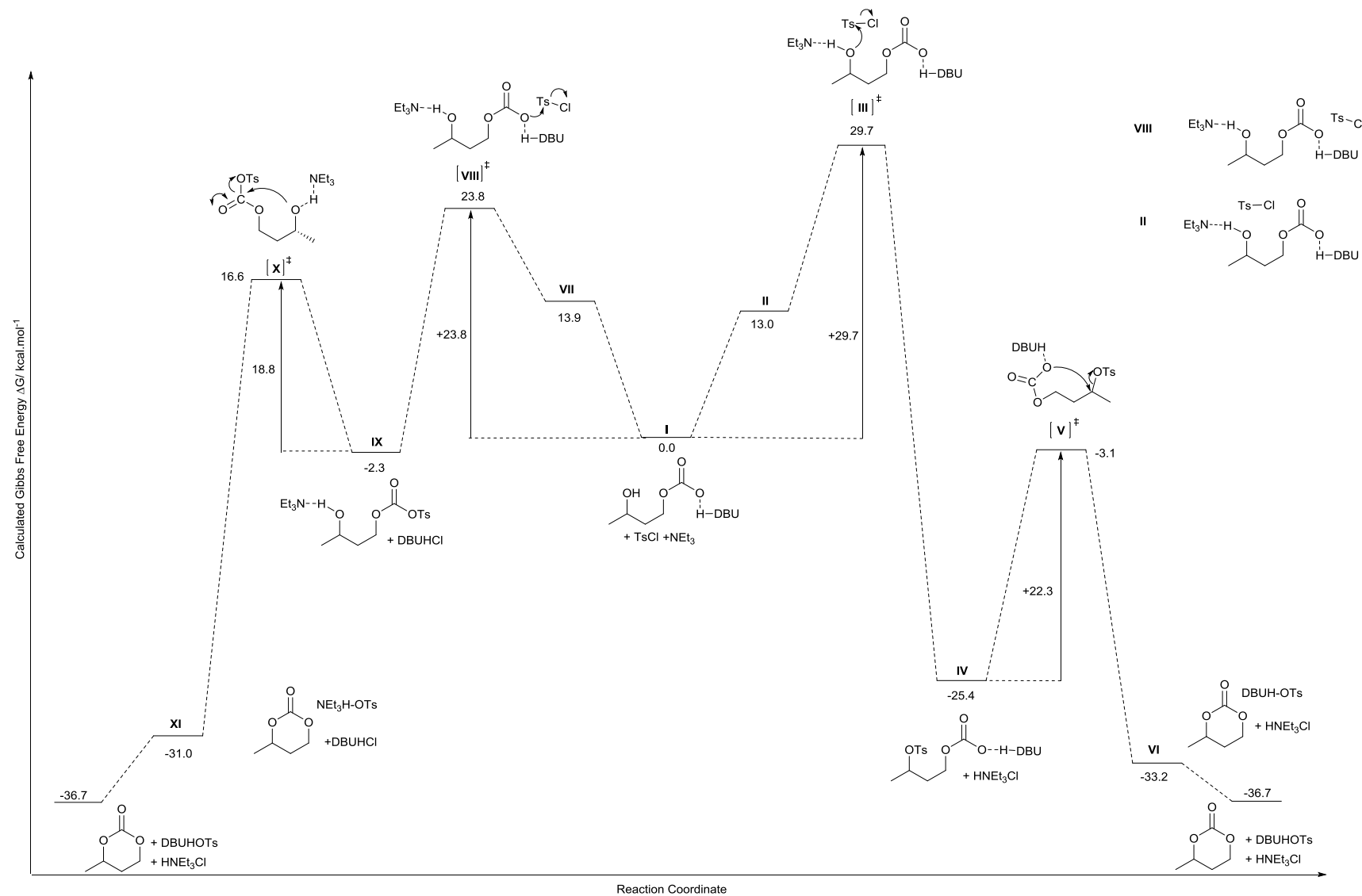


Figure S5: Computed energy diagram for the tosylation and subsequent cyclisation steps computed at the $\text{r}\omega\text{b97xd/6-31+g(d)/cpcm=chloroform/298K}$ level of theory.

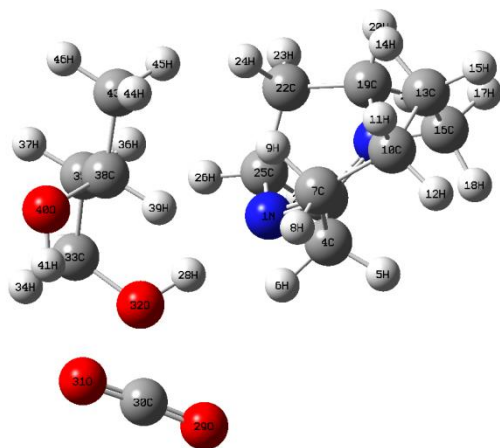
3.3 Optimised Geometries and Computed Gibbs Free Energies

Full coordinates for all calculated structures together with their 3 lowest calculated vibrations and their computed Gibbs Free Energies are reported below. They are also available via the corresponding Gaussian 09 output files, stored in the digital repositories:

<http://dx.doi.org/10.6084/m9.figshare.1333535> (for structures related to Figure S4)

<http://dx.doi.org/10.6084/m9.figshare.1333544> (for structures related to Figure S5)

A



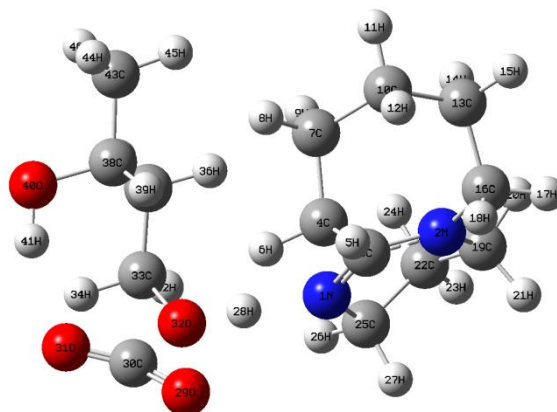
0	1			
N	0.58213100	1.01084300	-1.14937900	
N	2.73553700	0.26358800	-0.54831800	
C	1.42240000	0.06677600	-0.85142900	
C	0.89280100	-1.34709800	-0.79400900	
H	1.39561000	-1.97293400	-1.54329000	
H	-0.15726800	-1.29030400	-1.08821800	
C	1.01499500	-2.00011600	0.59568200	
H	0.25702600	-2.78897000	0.66452400	
H	0.76418300	-1.25971100	1.36586100	
C	2.38383100	-2.61269000	0.90057000	
H	2.33550100	-3.12409100	1.86944700	
H	2.59932400	-3.38614000	0.14929400	
C	3.53944800	-1.61127200	0.91927500	
H	3.41109900	-0.89258400	1.73998400	
H	4.47583300	-2.14980100	1.10938800	
C	3.68714400	-0.83451800	-0.39152200	
H	4.68197100	-0.38387600	-0.44780800	
H	3.61167700	-1.51669800	-1.24665700	
C	3.26098700	1.60331400	-0.28161000	
H	3.88276400	1.55172400	0.61985400	
H	3.90950200	1.91202800	-1.11270800	
C	2.13062900	2.60081300	-0.08843300	
H	2.52889800	3.61933900	-0.11864300	
H	1.66197400	2.45161200	0.89228300	
C	1.09085000	2.37457500	-1.18055300	

H	0.24485600	3.06105900	-1.06245300
H	1.53673200	2.58469400	-2.16455100
H	-1.16928800	0.86549100	-1.23034900
O	-2.57659600	-1.86108700	-2.34834200
C	-3.29107300	-1.54858000	-1.48527000
O	-4.04845100	-1.31228900	-0.62844100
O	-2.16609300	0.82227600	-1.21835200
C	-2.65804900	1.74911200	-0.26680400
H	-3.71568700	1.50466100	-0.11059700
C	-1.90234500	1.71707000	1.06115600
H	-0.88390300	2.09302100	0.90345100
H	-2.39680800	2.40168600	1.76373500
C	-1.80509900	0.33074400	1.69582200
H	-1.33305900	-0.35002900	0.97497400
O	-3.09699300	-0.18539900	2.03380600
H	-3.54316100	-0.44709200	1.21617100
H	-2.62230700	2.77117100	-0.67330800
C	-0.98036600	0.35149700	2.97118600
H	-0.89657100	-0.65395300	3.39644000
H	0.02881700	0.72472800	2.76594300
H	-1.44325500	1.00819200	3.71739500

Sum of electronic and thermal Free Energies= -958.994080

Frequencies -- 20.7556 26.9096 29.6649

TS_{AB}



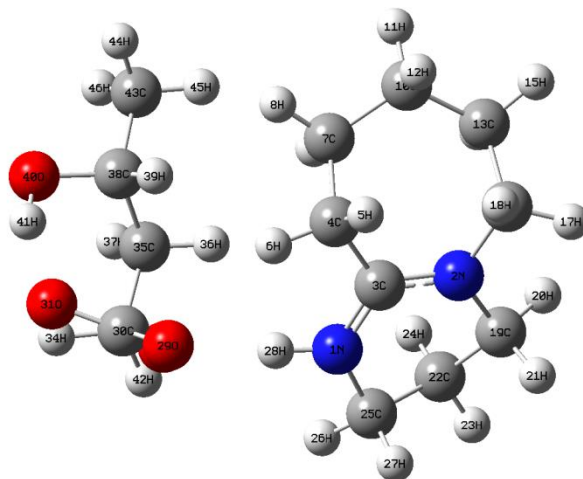
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H	1.29717500	0.67679200	2.19593200
H	-0.18357600	0.35260200	1.31574100
C	0.98575000	1.98332900	0.48617200
H	0.17742800	2.62509600	0.85455600
H	0.81250100	1.84840800	-0.58976900
C	2.31721600	2.70326700	0.71247400
H	2.27483400	3.68606300	0.22851000
H	2.43534300	2.88990400	1.78935900

C	3.55044500	1.95018500	0.20988200
H	3.52171000	1.85194800	-0.88351500
H	4.44578800	2.53405600	0.45480500
C	3.70404000	0.55538400	0.82197700
H	4.73009000	0.20101400	0.69545300
H	3.52145800	0.58838500	1.90198700
C	3.50124900	-1.36280000	-0.74428700
H	4.22020000	-0.77552500	-1.32520700
H	4.06418900	-2.12364200	-0.18843200
C	2.48336900	-2.01213700	-1.66751100
H	2.95764300	-2.82741500	-2.22109300
H	2.11592100	-1.27832400	-2.39467800
C	1.31662500	-2.52029500	-0.83066500
H	0.53284800	-2.94583400	-1.46508400
H	1.65776900	-3.31925500	-0.15699400
H	-0.71885300	-1.42359100	0.04662500
O	-1.93908600	-1.51942000	2.46463400
C	-2.74321900	-1.23600700	1.64069000
O	-3.83683200	-0.89629400	1.30618700
O	-1.80062600	-1.47344900	0.02544900
C	-2.33143300	-1.09595200	-1.23654500
H	-3.41598700	-1.23638900	-1.18051200
C	-1.98809200	0.33263900	-1.64864700
H	-0.89717800	0.43257100	-1.72140000
H	-2.39689000	0.49705900	-2.65519000
C	-2.52228500	1.42536300	-0.71821600
H	-2.04186200	1.32325400	0.26645800
O	-3.93697600	1.33065100	-0.55108700
H	-4.11798200	0.57380400	0.02809700
H	-1.95234100	-1.79652200	-1.99102200
C	-2.23182100	2.81423100	-1.26386100
H	-2.57288800	3.58175200	-0.56211600
H	-1.15915800	2.95123000	-1.43120400
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Sum of electronic and thermal Free Energies= -958.983371

Frequencies -- -347.0735 17.2581 33.9212

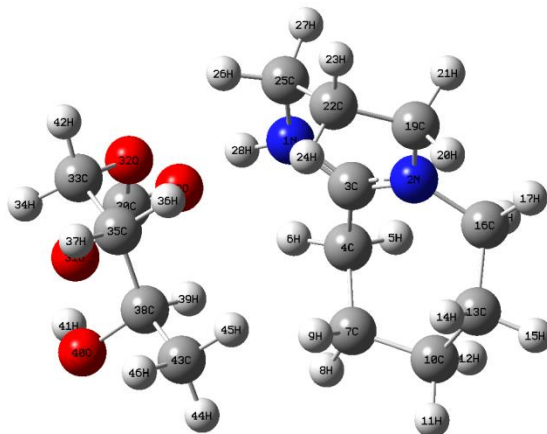
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H	-0.08972600	0.15811200	1.49568500
C	0.81679900	1.90778200	0.56406000
H	-0.02109000	2.45798700	1.00445100
H	0.56261700	1.73982700	-0.49010100
C	2.07780000	2.76782000	0.67072500
H	1.89036600	3.72914700	0.17944300
H	2.26250600	2.98913000	1.73102000
C	3.33987500	2.14191000	0.07371000
H	3.23094300	2.01195500	-1.01069300
H	4.18060400	2.82692000	0.22990100
C	3.71077700	0.79486500	0.69650500
H	4.75346900	0.55144500	0.48561100
H	3.61170000	0.82615000	1.78635800
C	3.60855700	-1.24698400	-0.74986200
H	4.29465900	-0.64811700	-1.35341300
H	4.20260800	-1.95236200	-0.15819500
C	2.61887000	-1.97267900	-1.64758900
H	3.14048200	-2.75675300	-2.20110500
H	2.19164800	-1.27118100	-2.37222700
C	1.50759700	-2.57311900	-0.80163500
H	0.69957400	-2.96676800	-1.42071600
H	1.88627200	-3.38689700	-0.17369300
H	-0.05805400	-1.54624900	0.23785800
O	-1.80161000	-1.46361200	2.37169300
C	-2.52474100	-1.22356400	1.39052500
O	-3.69834300	-0.78945900	1.34708500
O	-1.88412100	-1.49535900	0.17216200
C	-2.54592600	-1.22858100	-1.06826500
H	-3.62411300	-1.33774600	-0.93041300
C	-2.18868500	0.14117300	-1.63329800
H	-1.10539800	0.18705500	-1.80829600
H	-2.67844200	0.23284700	-2.61256000
C	-2.60124700	1.33083000	-0.75930100
H	-2.02100300	1.29735200	0.17620200
O	-3.98629600	1.28699400	-0.43639300
H	-4.09048500	0.55323300	0.20581900
H	-2.20472700	-2.00986200	-1.75274800
C	-2.32633100	2.65532500	-1.45283200
H	-2.58868100	3.49205100	-0.79767200
H	-1.26810900	2.74543200	-1.71931400
H	-2.91908100	2.73272600	-2.37186500
Sum of electronic and thermal Free Energies=			-959.014418
Frequencies --	20.9617	35.7004	47.5288

TS_{BC}



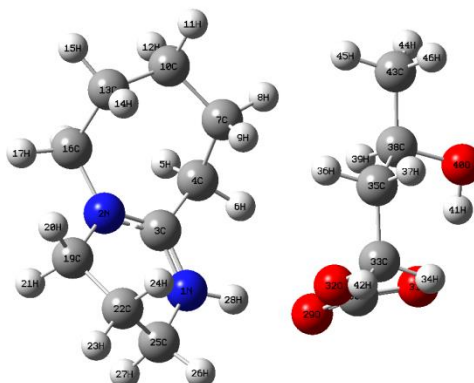
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C	1.16578600	-0.79525700	-1.44056300	
H	1.85765000	-0.89349400	-2.28576700	
H	0.16472700	-0.69101900	-1.86834100	
C	1.24450300	-2.04743300	-0.54515200	
H	0.64218900	-2.82774100	-1.02141000	
H	0.77349900	-1.83630700	0.42258400	
C	2.66182800	-2.57950300	-0.32645400	
H	2.60519500	-3.50549600	0.25670100	
H	3.09376000	-2.84880100	-1.30027100	
C	3.60705700	-1.60465800	0.37821400	
H	3.25916000	-1.40066300	1.39911800	
H	4.59528100	-2.06976000	0.46599000	
C	3.78185600	-0.27629400	-0.35885400	
H	4.67641600	0.23875100	-0.00501500	
H	3.91869200	-0.43969600	-1.43280600	
C	2.94762700	1.83072000	0.70199100	
H	3.59603300	1.49114100	1.51307200	
H	3.49975800	2.57100600	0.11216800	
C	1.66419200	2.41953200	1.26502800	
H	1.88594500	3.36802400	1.75889600	
H	1.23967500	1.73873300	2.01124200	
C	0.66720900	2.63006100	0.13721200	
H	-0.31767800	2.91504400	0.51245600	
H	1.00881400	3.41097400	-0.55089500	
H	-0.40799000	1.16165900	-0.96153800	
O	-1.87103800	0.13070100	-2.64043400	
C	-2.63601800	0.12762500	-1.65792500	
O	-3.57475400	-0.65120600	-1.37926100	
O	-2.34882300	1.16398400	-0.76104200	
C	-3.03608500	1.22704400	0.49191200	
H	-4.03255300	0.79392300	0.37716800	
C	-2.25404800	0.53742800	1.60498000	
H	-1.29659000	1.05374000	1.75291800	
H	-2.82499500	0.64509600	2.53697000	
C	-1.97284000	-0.94753300	1.35888300	
H	-1.35208000	-1.03838200	0.45356000	
O	-3.17440200	-1.68276400	1.16019100	

H	-3.50990500	-1.42250400	0.27714600
H	-3.14491700	2.29204000	0.71358900
C	-1.21952700	-1.57491800	2.51980900
H	-1.00623100	-2.62883200	2.31403800
H	-0.26924600	-1.05601000	2.68802400
H	-1.81229600	-1.51361700	3.44000400

Sum of electronic and thermal Free Energies= -959.013594

Frequencies -- -53.8608 18.3737 40.1915

C



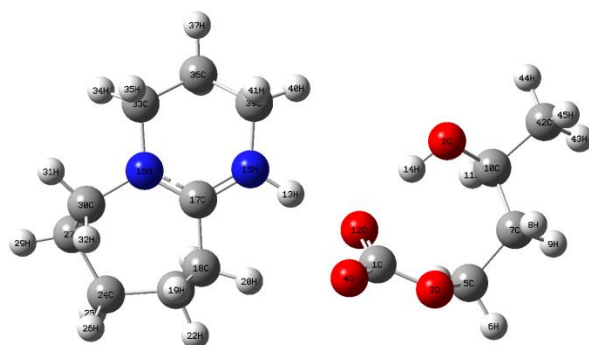
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C	-1.09049700	0.60922700	-1.51848700
H	-1.73109800	0.93907000	-2.34497800
H	-0.23737300	0.09331300	-1.96493900
C	-0.60134400	1.82253300	-0.70432200
H	0.22574400	2.27761700	-1.25928900
H	-0.18243400	1.46985300	0.24663100
C	-1.66204000	2.89428200	-0.44930000
H	-1.19000700	3.73729500	0.06828400
H	-2.01342700	3.27976300	-1.41666100
C	-2.87163100	2.42501200	0.36090600
H	-2.57135200	2.14606400	1.37923400
H	-3.58044400	3.25554900	0.45379200
C	-3.61087200	1.24810500	-0.27652200
H	-4.61210700	1.15277500	0.14783900
H	-3.74148900	1.40520500	-1.35214000
C	-3.58983500	-0.94456000	0.92638400
H	-3.97821600	-0.31952100	1.73449700
H	-4.43855000	-1.44621500	0.44720300
C	-2.59134300	-1.95158000	1.47341500
H	-3.11879100	-2.69349500	2.07730200
H	-1.86479200	-1.44307500	2.11659300
C	-1.86631300	-2.62288400	0.31780800
H	-1.03662100	-3.24070500	0.66659700
H	-2.54875300	-3.25791600	-0.25808600
H	-0.37676400	-1.77164700	-0.97113600
O	1.19506400	-2.06499100	-1.63121000

C	2.10142400	-1.69618500	-0.84301700
O	3.31157300	-1.51362700	-1.09696900
O	1.64020400	-1.48783100	0.44118600
C	2.54041100	-1.00981600	1.44334100
H	3.55288000	-1.35958900	1.22664000
C	2.49001900	0.50761300	1.57998800
H	1.47573700	0.80466500	1.87710500
H	3.16443200	0.79414200	2.39853800
C	2.88466700	1.28165300	0.31798700
H	2.16529900	1.04190200	-0.47931500
O	4.18924900	0.92453300	-0.12659800
H	4.10511700	0.02389700	-0.50226600
H	2.20718500	-1.47488500	2.37481300
C	2.85749100	2.78302300	0.55210700
H	3.10204600	3.31937700	-0.37033900
H	1.86419400	3.10401100	0.88465400
H	3.58561800	3.06387200	1.32209900

Sum of electronic and thermal Free Energies= -959.018545

Frequencies -- 15.9275 31.0701 35.0222

D



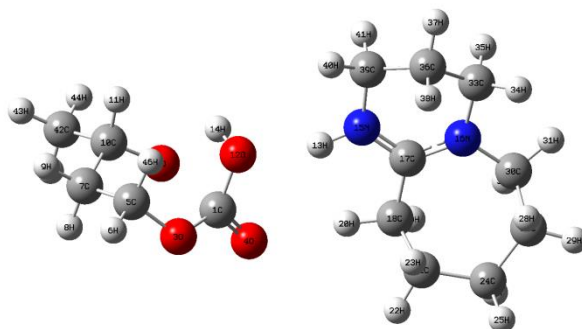
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O	3.09375400	-1.84133200	0.85730300
O	1.22452700	-1.59513100	2.00301900
C	3.84117600	-1.69879000	-0.35798700
H	4.38231300	-2.64441900	-0.44344000
C	4.84543100	-0.54309300	-0.34622300
H	5.25192600	-0.42663000	0.66717800
H	5.68253800	-0.84446200	-0.98981100
C	4.34757100	0.81289500	-0.85982800
H	3.91342100	0.65821200	-1.86165900
O	1.44350900	-0.54161500	0.02593200
H	-0.05990300	0.24245400	0.33463200
H	2.58975200	0.78828200	-0.01357100
N	-0.94193200	0.78117200	0.42752000
N	-3.25493900	0.74486300	0.40549600
C	-2.08221700	0.12201000	0.36284500
C	-2.01163000	-1.37026700	0.19806200
H	-2.55008100	-1.85053400	1.02362000
H	-0.96382300	-1.66012200	0.29889900
C	-2.56901500	-1.85083100	-1.15539900

H	-2.14642400	-2.84204300	-1.34886400
H	-2.20025000	-1.19177000	-1.95173100
C	-4.09538500	-1.94919100	-1.21042500
H	-4.38815300	-2.34666500	-2.18882600
H	-4.42693900	-2.68373300	-0.46335200
C	-4.83818500	-0.63389200	-0.96532000
H	-4.61397600	0.09149100	-1.75801100
H	-5.91642800	-0.82536200	-1.00548900
C	-4.52637200	0.00659800	0.38858500
H	-5.29692000	0.73278300	0.65246800
H	-4.51983600	-0.74503200	1.18487200
C	-3.34073800	2.21279600	0.43537600
H	-4.20558100	2.50150900	-0.16689600
H	-3.52342100	2.53212200	1.46782400
C	-2.07689300	2.84924200	-0.12213400
H	-2.10468200	3.92631600	0.05794000
H	-2.02548200	2.68691500	-1.20408700
C	-0.85796500	2.23089700	0.54415500
H	0.06849500	2.54995000	0.06297400
H	-0.80582100	2.50860200	1.60294100
C	5.48855300	1.81310100	-0.97196200
H	6.25486800	1.45359200	-1.66654900
H	5.11563900	2.77541600	-1.33729000
H	5.95545400	1.97137700	0.00760800
H	3.15273800	-1.61635200	-1.20429400

Sum of electronic and thermal Free Energies= -959.013651

Frequencies -- 17.3960 19.0715 28.1213

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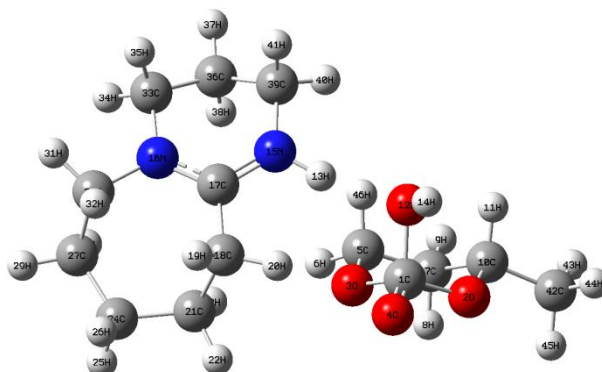
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O	-2.94853800	-1.21009200	1.22344100
O	-1.43948300	-1.63296700	-0.34003200
C	-3.97626600	-0.31859600	1.68570700
H	-4.33849300	-0.78074700	2.60622800
C	-5.08276700	-0.18110900	0.65490900
H	-5.44687300	-1.18299400	0.38674400
H	-5.91793500	0.36200400	1.11762700
C	-4.60155000	0.55516800	-0.60329500
H	-4.39908000	1.60434500	-0.28418600
O	-1.64007800	0.50441400	0.40398100
H	0.19411700	0.65631800	0.05720900

H	-2.12822600	0.93178800	-0.33772600
N	1.13503900	1.05439400	-0.01293500
N	3.38341400	0.72756700	-0.42532100
C	2.13897300	0.27145700	-0.36909700
C	1.83232900	-1.16688800	-0.66976000
H	2.16509600	-1.39944800	-1.68844400
H	0.74567700	-1.28926700	-0.65355000
C	2.47987700	-2.13513100	0.33961000
H	1.92277600	-3.07636200	0.29050600
H	2.34096700	-1.74224600	1.35496700
C	3.95943200	-2.42918600	0.08028100
H	4.30755000	-3.16245300	0.81657800
H	4.05539000	-2.90657500	-0.90490200
C	4.88003400	-1.20765300	0.12227700
H	4.89929700	-0.77057800	1.12886900
H	5.90308700	-1.52795300	-0.10478400
C	4.49863100	-0.11704200	-0.87982200
H	5.33760900	0.56113600	-1.04420300
H	4.25143300	-0.54999600	-1.85447400
C	3.72413800	2.09423800	-0.00013400
H	4.69550700	2.04656300	0.49775000
H	3.82906600	2.72168700	-0.89235400
C	2.67525400	2.65369700	0.94778500
H	2.86902000	3.71532800	1.11634700
H	2.73343800	2.13994200	1.91313500
C	1.29281000	2.45841100	0.34654100
H	0.50403800	2.70876100	1.05801500
H	1.16089900	3.08002700	-0.54590200
C	-5.71258400	0.62222600	-1.65349300
H	-6.60858000	1.12280200	-1.26290400
H	-5.36678900	1.17254800	-2.53618100
H	-5.99173700	-0.39100600	-1.97090300
H	-3.53247000	0.65249200	1.92996600

Sum of electronic and thermal Free Energies= -958.946382

Frequencies -- -342.3582 14.4149 16.9010

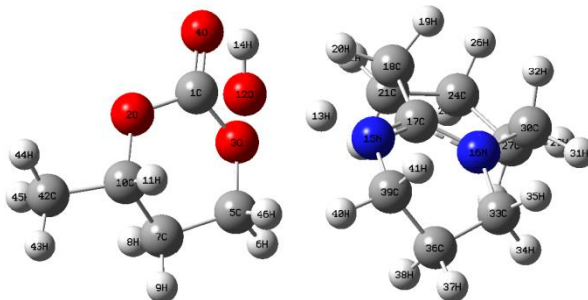
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0 1			
C	-2.19119000	-0.72725900	-0.81455300
O	-3.59100800	-0.65508700	-0.49383500
O	-1.43592800	-0.75110100	0.40259000

O	-1.92757400	-1.71312000	-1.57651100
C	-1.71110400	0.28198700	1.33818300
H	-1.09602600	0.06324900	2.21580000
C	-3.19257800	0.31377500	1.68056400
H	-3.46611600	-0.59734600	2.22880400
H	-3.41595800	1.17671400	2.31883800
C	-4.00043800	0.38954600	0.38901100
H	-3.80298400	1.35603400	-0.09754900
O	-1.83637700	0.58053100	-1.41167900
H	-0.08619000	0.80384000	-1.10439300
H	-2.00809200	0.45726100	-2.35491100
N	0.85454500	1.13592600	-0.84747400
N	3.00807500	0.60681700	-0.20320200
C	1.80948700	0.24585800	-0.64970300
C	1.49319100	-1.19711700	-0.91894100
H	2.17106600	-1.57034900	-1.69681400
H	0.47611900	-1.25366000	-1.31495300
C	1.58691900	-2.07733900	0.34112000
H	0.98884000	-2.97442200	0.15057800
H	1.10244100	-1.55656300	1.17546700
C	3.00621700	-2.50405900	0.71924100
H	2.95591600	-3.18006600	1.58068200
H	3.43291500	-3.08664800	-0.10940500
C	3.95844600	-1.35261000	1.04648700
H	3.62373300	-0.81628200	1.94387000
H	4.94876300	-1.76451500	1.27172200
C	4.11988800	-0.34953500	-0.09610800
H	5.01808200	0.25267700	0.05215600
H	4.24480500	-0.86561800	-1.05385800
C	3.29112300	1.98797200	0.21474200
H	3.94094600	1.93635800	1.09197000
H	3.84327100	2.49097800	-0.58758600
C	2.01094200	2.73543700	0.55073800
H	2.23655200	3.79345400	0.70181600
H	1.58160900	2.34271700	1.47892900
C	1.01464400	2.55952100	-0.58365800
H	0.03262600	2.96199400	-0.32704000
H	1.36254900	3.06403800	-1.49206100
C	-5.49411800	0.23340300	0.61179200
H	-5.86375000	1.02835900	1.26890200
H	-6.03487500	0.29048400	-0.33855400
H	-5.71309500	-0.73294300	1.08043700
H	-1.39295300	1.25378400	0.93388400
Sum of electronic and thermal Free Energies=			-958.970665
Frequencies --	21.0858	29.5667	37.7718

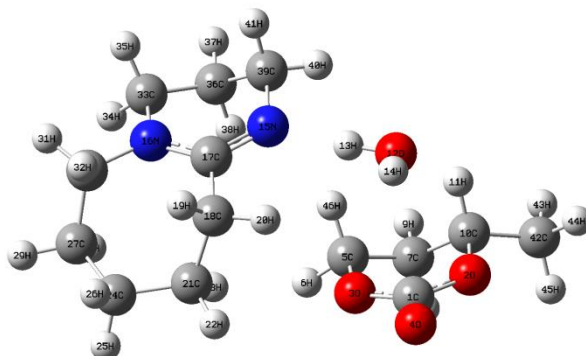
TS_{EF}



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C	-2.28209600	-1.12332100	-0.53670300	
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O	-1.45929400	-0.93885500	0.53791600	
O	-2.07665200	-2.10098600	-1.25312400	
C	-1.60518000	0.24476300	1.32405900	
H	-1.01410900	0.06559800	2.22435200	
C	-3.06461300	0.50991800	1.63648400	
H	-3.45953100	-0.26402100	2.30625200	
H	-3.16759400	1.47933100	2.13538600	
C	-3.84192500	0.51148700	0.33038500	
H	-3.48536500	1.32844000	-0.30662500	
O	-1.63465100	0.44609800	-1.60944300	
H	-0.18467100	0.76218400	-1.26641800	
H	-1.65444700	-0.01046600	-2.45996100	
N	0.79197800	1.12036900	-0.95569200	
N	2.93462900	0.66627500	-0.19815500	
C	1.75971600	0.27055900	-0.69522900	
C	1.49640200	-1.18841500	-0.94879200	
H	2.19016200	-1.55005400	-1.71855800	
H	0.48640800	-1.27009000	-1.35588300	
C	1.60229900	-2.05989600	0.31618800	
H	1.03515600	-2.97669200	0.12436700	
H	1.09328500	-1.55121800	1.14334200	
C	3.02770200	-2.44171700	0.71817200	
H	2.98320800	-3.12684100	1.57286000	
H	3.49176700	-3.00141600	-0.10633000	
C	3.92884900	-1.25878300	1.07378400	
H	3.55049500	-0.73915900	1.96371100	
H	4.92824400	-1.63391700	1.32292600	
C	4.07636100	-0.24736000	-0.06330200	
H	4.94836200	0.38770400	0.10602700	
H	4.24439000	-0.75930200	-1.01711000	
C	3.15652800	2.04956700	0.24448300	
H	3.73895600	2.00765800	1.16932800	
H	3.75745700	2.57092900	-0.51010000	
C	1.83858500	2.76850400	0.48269300	
H	2.02738700	3.83353800	0.63726400	
H	1.35532000	2.37454800	1.38383900	
C	0.93022500	2.54886800	-0.71714700	
H	-0.07015000	2.95516100	-0.54879200	
H	1.34368700	3.03455000	-1.60938500	
C	-5.34413800	0.59429200	0.51238600	
H	-5.60501500	1.53700200	1.00456000	
H	-5.85358800	0.55770600	-0.45554800	

H	-5.70723800	-0.23323100	1.13186000
H	-1.16834600	1.08583200	0.77637600
Sum of electronic and thermal Free Energies=			-958.961071
Frequencies --	-330.3843	24.1831	26.1442

F



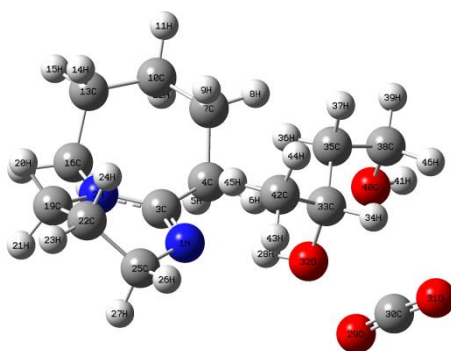
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O	3.74456000	-0.58997300	0.22946700
O	1.63939300	-1.21358600	-0.47366200
O	2.76809600	-2.41845700	0.98424200
C	1.45987300	-0.00314000	-1.24229900
H	0.85028100	-0.30377300	-2.09536500
C	2.79102200	0.57873800	-1.65647000
H	3.28674700	-0.06054500	-2.39650900
H	2.63281500	1.56344800	-2.10628000
C	3.65312900	0.70974000	-0.41813400
H	3.16874500	1.36991200	0.30817800
O	1.62892200	0.60168900	2.13842400
H	0.70999200	0.72757200	1.77175200
H	1.56743300	-0.15396700	2.73508700
N	-0.85039900	1.12754400	1.04968900
N	-2.99407000	0.67418900	0.17936200
C	-1.81802900	0.31071700	0.76265500
C	-1.60050000	-1.15659600	1.05088100
H	-2.33793500	-1.51602300	1.78086400
H	-0.62018400	-1.23358400	1.52511200
C	-1.63159400	-2.04817100	-0.20454500
H	-1.06264900	-2.95802500	0.01684000
H	-1.09839100	-1.54129800	-1.01891000
C	-3.03216800	-2.45296400	-0.66986900
H	-2.94070000	-3.15229800	-1.50974800
H	-3.52703100	-3.00492600	0.14247700
C	-3.92982300	-1.28580400	-1.08390500
H	-3.52087600	-0.78430700	-1.97130200
H	-4.91570500	-1.67718800	-1.36321100
C	-4.11862100	-0.24602900	0.02339500
H	-4.99236500	0.37457800	-0.19413000
H	-4.32616300	-0.74282700	0.97851100
C	-3.17619500	2.00912400	-0.39185200
H	-3.66816900	1.89740500	-1.36486700
H	-3.84570900	2.59529700	0.25231200

C	-1.83909800	2.71325500	-0.55197400
H	-2.00357700	3.77125600	-0.77678500
H	-1.28304600	2.27313900	-1.38883300
C	-1.03838200	2.53641200	0.73355600
H	-0.05003000	3.00034200	0.64295400
H	-1.55355100	3.04167300	1.56465500
C	5.07506000	1.15253700	-0.68670000
H	5.06644600	2.15529200	-1.12518900
H	5.65089200	1.18672100	0.24266700
H	5.56921600	0.46974000	-1.38561900
H	0.88594800	0.68422900	-0.61518000

Sum of electronic and thermal Free Energies= -958.987090

Frequencies -- 18.9117 32.6910 35.1002

A'



0 1

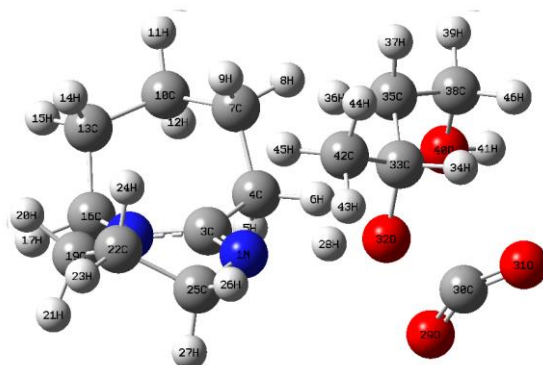
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C	1.47426200	0.20041000	-0.61954800
C	0.97937900	-1.22619000	-0.63191800
H	1.31753600	-1.73723400	-1.54350400
H	-0.11057100	-1.17856000	-0.67796400
C	1.40431400	-2.03938900	0.60537900
H	0.68187600	-2.85364800	0.73446900
H	1.32160000	-1.40688400	1.50001800
C	2.81020700	-2.63984900	0.52881100
H	2.98200100	-3.26248600	1.41525700
H	2.85769600	-3.31322600	-0.33933000
C	3.93691200	-1.61162800	0.41505600
H	3.99189300	-1.00351000	1.32821900
H	4.89408300	-2.13989200	0.32544500
C	3.78891900	-0.67568100	-0.78749800
H	4.74641500	-0.19153700	-0.99957300
H	3.53066600	-1.24944800	-1.68552700
C	3.38940100	1.71446400	-0.27822800
H	4.19653200	1.57113100	0.44996800
H	3.83542800	2.14622100	-1.18456400
C	2.32667500	2.64281300	0.28643300
H	2.70347100	3.67007500	0.29854000
H	2.09075500	2.36005900	1.31989200
C	1.06923200	2.51809200	-0.56663300
H	0.26819100	3.15564700	-0.17738500
H	1.28235700	2.86144300	-1.59071400

H	-1.17480400	1.04031900	-0.31155800
O	-2.96363900	-0.27730100	-2.54776200
C	-3.75909600	-0.19137900	-1.69926200
O	-4.64177400	-0.11678900	-0.94050300
O	-2.14609400	1.12771700	-0.11556900
C	-2.33644100	0.99412800	1.28266500
H	-3.41984500	1.08309000	1.43775300
C	-1.88316600	-0.37022800	1.81664300
H	-0.82245600	-0.51829400	1.57932100
H	-1.95971000	-0.34122700	2.91191000
C	-2.68115300	-1.58081300	1.35632500
H	-2.43374000	-2.43487600	2.00108900
O	-2.37437400	-1.90738200	0.00199500
H	-2.79670300	-2.75056200	-0.20454600
C	-1.63573800	2.12853300	2.03315300
H	-1.94627200	3.09731300	1.62800300
H	-1.87564800	2.10587900	3.10244000
H	-0.54781600	2.04157700	1.92261000
H	-3.75761400	-1.37980100	1.45840200

Sum of electronic and thermal Free Energies= -958.987274

Frequencies -- 23.4170 34.2598 40.1588

TS_{AB}'



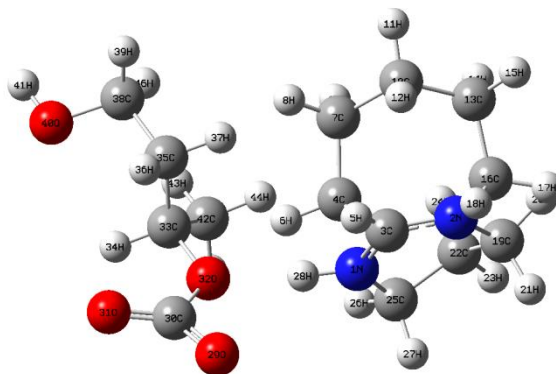
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N	-0.43281200	-1.15561000	-0.38775900
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C	-1.37419500	-0.26603600	-0.52335300
C	-0.95746500	1.17210200	-0.69524000
H	-1.33982000	1.56447900	-1.64674200
H	0.13171700	1.18697000	-0.76262800
C	-1.41173400	2.08107000	0.46185300
H	-0.73586400	2.94326800	0.49150300
H	-1.27895000	1.55020200	1.41452500
C	-2.85184300	2.58697800	0.34950100
H	-3.05300900	3.28293100	1.17274900
H	-2.94785000	3.16669300	-0.57982900
C	-3.91651100	1.48815500	0.35100900
H	-3.92860200	0.96695400	1.31767400
H	-4.90317400	1.95040300	0.22572200
C	-3.72762700	0.45352800	-0.76154000
H	-4.65742500	-0.10035400	-0.91557200
H	-3.50707300	0.95207600	-1.71232100

C	-3.18800800	-1.85966600	-0.04300900
H	-4.02066200	-1.69584200	0.64984500
H	-3.57995800	-2.40607700	-0.91070500
C	-2.08301500	-2.65140400	0.63680800
H	-2.39667500	-3.69214000	0.75860300
H	-1.88603200	-2.23919600	1.63378400
C	-0.82002700	-2.54748400	-0.20825500
H	0.01567800	-3.07445300	0.26277200
H	-0.98653200	-3.01704100	-1.18877200
H	1.04810200	-0.90304600	-0.29232900
O	2.34759000	-0.31545600	-2.47652500
C	3.09423900	-0.29992500	-1.54320300
O	4.19848300	-0.13061000	-1.11925300
O	2.10518400	-0.89758400	-0.15468200
C	2.49251000	-0.62711700	1.19516100
H	3.58752300	-0.65125800	1.18566300
C	2.02521300	0.74835800	1.67827800
H	0.93760200	0.82814100	1.56021000
H	2.22931100	0.80453300	2.75509100
C	2.69960800	1.94890500	1.03327000
H	2.47635000	2.84819300	1.62340200
O	2.22209600	2.11941700	-0.29787900
H	2.72760000	2.82812500	-0.71441800
C	1.96914800	-1.74447600	2.09238700
H	2.26476600	-2.72079600	1.69616800
H	2.37730000	-1.64229400	3.10340200
H	0.87541200	-1.70986300	2.15937500
H	3.78892300	1.80501300	1.02843800

Sum of electronic and thermal Free Energies= -958.974844

Frequencies -- -247.5088 23.2284 39.0968

B'



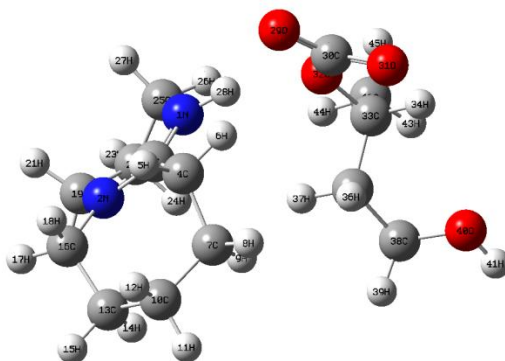
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C	1.69660200	-0.35737900	0.35650700
C	1.07994300	0.74690300	1.16759400
H	1.57775200	0.80552000	2.14255600
H	0.04140100	0.47235100	1.36374100
C	1.14397600	2.11005400	0.45083800
H	0.36412700	2.74487400	0.88409600

H	0.88635200	1.97473800	-0.60760900
C	2.48925900	2.82938600	0.57480900
H	2.40743300	3.81090300	0.09450600
H	2.69082200	3.01726900	1.63845700
C	3.67921100	2.07821300	-0.02635300
H	3.56194500	1.97377000	-1.11261500
H	4.58988800	2.66373800	0.14199000
C	3.89559000	0.69180800	0.58129200
H	4.90473200	0.33478700	0.36859000
H	3.79880500	0.72351800	1.67144300
C	3.56965700	-1.31499200	-0.88105800
H	4.31169700	-0.78998200	-1.48734800
H	4.08980400	-2.08101800	-0.29488700
C	2.50430300	-1.93260400	-1.77342100
H	2.93888000	-2.76425800	-2.33229500
H	2.14500800	-1.18961900	-2.49361600
C	1.34435900	-2.41834900	-0.91908600
H	0.49475100	-2.72683900	-1.53166000
H	1.64326400	-3.26803000	-0.29518500
H	-0.09213300	-1.27092900	0.18739500
O	-1.42854800	-1.67727100	2.50726400
C	-2.31386500	-1.22243100	1.75520300
O	-3.49060300	-0.89985900	1.99539900
O	-1.85502000	-1.08056400	0.42839600
C	-2.67276800	-0.41267900	-0.54459200
H	-3.71555800	-0.66839400	-0.34509700
C	-2.47403800	1.09716400	-0.39869200
H	-2.67338400	1.37601700	0.64259600
H	-1.42380500	1.33788600	-0.60828400
C	-3.34337700	1.94435600	-1.31212700
H	-3.12557700	3.00577600	-1.13579900
O	-4.71305000	1.66825200	-1.02734500
H	-5.26305500	2.21506700	-1.60154800
C	-2.24956400	-0.95137700	-1.90285400
H	-2.88893600	-0.54930600	-2.69488400
H	-1.21154100	-0.67754400	-2.12909200
H	-2.33607400	-2.04232700	-1.92155500
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Sum of electronic and thermal Free Energies= -959.008702

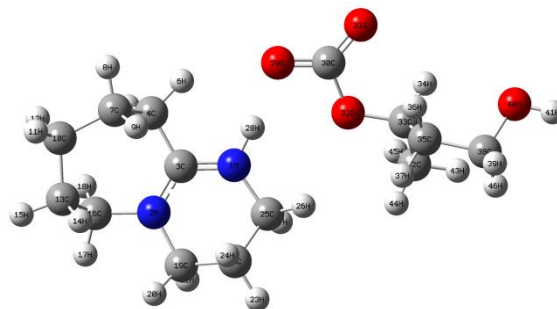
Frequencies -- 14.8829 26.3162 33.5021

TS_{BC}



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C	1.66644600	-0.44523700	0.56944100
C	1.38041400	0.78081200	1.38831200
H	2.14412900	0.87642300	2.16972000
H	0.43021300	0.61762300	1.90243900
C	1.32364300	2.06674900	0.54075900
H	0.74541100	2.80373800	1.10741700
H	0.76221800	1.87149200	-0.38127900
C	2.69141500	2.66508700	0.20570900
H	2.54151200	3.61132300	-0.32619600
H	3.20757200	2.91203500	1.14386600
C	3.59887200	1.76091400	-0.63087900
H	3.15994900	1.58259100	-1.62099200
H	4.55575700	2.26966900	-0.79270000
C	3.89338000	0.41388900	0.03004600
H	4.76761900	-0.05254500	-0.42753800
H	4.12709600	0.54320000	1.09180500
C	3.01916500	-1.65866900	-1.06358400
H	3.55376700	-1.24022300	-1.91983700
H	3.66424800	-2.40936100	-0.59346100
C	1.70140800	-2.26891500	-1.51385200
H	1.90104900	-3.17787000	-2.08570800
H	1.16628400	-1.56812100	-2.16368800
C	0.84973300	-2.58597200	-0.29467700
H	-0.16075600	-2.89151200	-0.57163000
H	1.29914400	-3.38794500	0.30107700
H	-0.16338100	-1.19675700	0.96665800
O	-1.36143800	-0.61237700	2.90823200
C	-2.22559200	-0.23101300	2.08673500
O	-3.13746800	0.60443400	2.21372900
O	-2.08577300	-0.88634600	0.85280600
C	-2.80083400	-0.39329200	-0.28947600
H	-3.73566000	0.04708000	0.06355100
C	-1.93973300	0.68128600	-0.95710600
H	-1.72942200	1.46581400	-0.21954300
H	-0.97840100	0.23191900	-1.24039300
C	-2.54461300	1.31508900	-2.19718300
H	-1.84626800	2.06238200	-2.59670500
O	-3.77966000	1.93268300	-1.84303500
H	-4.15876500	2.33726900	-2.63296200
C	-3.09257900	-1.58556000	-1.18615300
H	-3.74193000	-1.29153300	-2.01692000
H	-2.16968400	-2.00346100	-1.60596700
H	-3.60389000	-2.36909700	-0.61855000
H	-2.70886900	0.55931400	-2.97717700
Sum of electronic and thermal Free Energies=			-959.005974
Frequencies --	-68.9678	22.3064	37.4527

C'

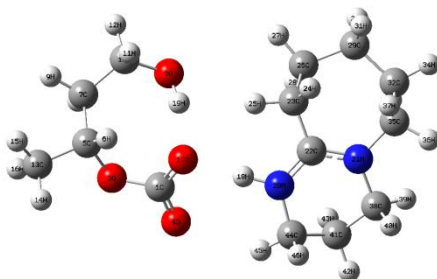


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C	-2.64462600	1.41424400	-0.48709200
H	-3.20517400	1.53958000	-1.42088700
H	-1.75248500	2.03899500	-0.56380800
C	-3.49858700	1.86371300	0.71448400
H	-3.45688500	2.95707900	0.75483700
H	-3.03707500	1.49918200	1.64116700
C	-4.96551000	1.43312100	0.64688100
H	-5.49581900	1.85405500	1.50859000
H	-5.42090100	1.87848200	-0.24865500
C	-5.19437900	-0.07930800	0.61181500
H	-4.85704800	-0.54368700	1.54743300
H	-6.27008600	-0.27175000	0.52948500
C	-4.50347800	-0.77767200	-0.56040600
H	-4.94170900	-1.76378100	-0.72484900
H	-4.64521500	-0.21532400	-1.48936600
C	-2.65201100	-2.39224800	-0.08297800
H	-3.43266200	-2.85808400	0.52348900
H	-2.59762800	-2.92863100	-1.03732800
C	-1.31966000	-2.43515900	0.64848600
H	-0.96144600	-3.46644400	0.69051500
H	-1.44978600	-2.07963200	1.67646000
C	-0.31290500	-1.55355200	-0.07289200
H	0.61011300	-1.43641300	0.49545200
H	-0.05328100	-1.97270900	-1.05178100
H	-0.25730700	0.59864500	-0.25084700
O	0.66903500	2.07135900	-0.21789500
C	1.90025600	1.80900000	-0.30914300
O	2.86512600	2.58791400	-0.24486500
O	2.12425000	0.45804000	-0.51788600
C	3.46921900	-0.04105000	-0.52505200
H	4.12055200	0.72486500	-0.95254900
C	3.88753000	-0.32554200	0.91942300
H	3.81294300	0.60569900	1.49291000
H	3.17593100	-1.03909000	1.35601400
C	5.28601400	-0.89686300	1.07909900
H	5.48891000	-1.06273900	2.14524400
O	6.22662500	0.02774900	0.53618200
H	7.11393700	-0.33504600	0.64809300
C	3.46265100	-1.27598200	-1.41249600
H	4.47818000	-1.66036800	-1.55021800
H	2.84835400	-2.07157100	-0.97458400

H	3.05767200	-1.02905100	-2.39878600
H	5.37099500	-1.86524100	0.56800200
Sum of electronic and thermal Free Energies=			-959.010334
Frequencies --	17.0642	21.4997	31.4471

D'



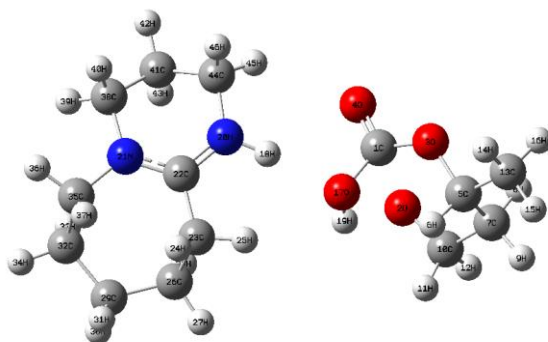
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O	-1.77006800	-2.21216300	-0.86990700
C	-4.24532400	-0.02397100	0.39377800
H	-3.69852600	0.09584100	1.33427700
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C	-3.19724400	2.30639000	-0.11539300
H	-3.06181300	2.48052200	0.96354900
H	-3.45737100	3.26619900	-0.57228900
C	-5.61828700	-0.62327700	0.66754100
H	-5.52041400	-1.60436600	1.14229200
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O	-1.57474600	-0.48519400	0.55838300
H	0.10329800	-0.95257000	0.50799700
H	-1.68735400	1.09209100	-0.24489400
N	1.10760100	-1.20358700	0.44448400
N	3.29853100	-0.46863100	0.38103600
C	2.00117900	-0.24102700	0.55823900
C	1.50125900	1.14485400	0.85828100
H	1.95457400	1.49897100	1.79174200
H	0.42662300	1.07426800	1.03788900
C	1.77625900	2.14456800	-0.28122200
H	1.07464800	2.97582600	-0.16075000
H	1.53621300	1.67097500	-1.24162900
C	3.20097300	2.70320200	-0.30383700
H	3.27493600	3.44579500	-1.10633300
H	3.38169500	3.24129400	0.63721100
C	4.30313000	1.65821200	-0.48820600
H	4.21774200	1.17453700	-1.46981100
H	5.27588300	2.16211400	-0.46429100
C	4.30779500	0.57799100	0.59486600
H	5.27072300	0.06462900	0.61737300
H	4.16652100	1.01976200	1.58690000

C	3.79446000	-1.77444600	-0.08110600
H	4.61209700	-1.58213400	-0.78054400
H	4.20321900	-2.31724600	0.77866800
C	2.69475100	-2.57214900	-0.76456200
H	3.04518100	-3.59175900	-0.94090500
H	2.45680500	-2.12193900	-1.73430200
C	1.45303900	-2.57958100	0.11286300
H	0.58890500	-3.01107600	-0.39455500
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Sum of electronic and thermal Free Energies= -959.012944

Frequencies -- 14.6545 24.8134 42.7061

TS_{DE}'

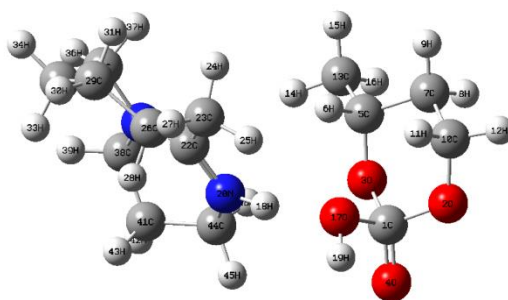


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H	-3.90532900	-3.10308500	0.86617000
C	-4.72062900	-1.44765400	-0.23795600
H	-4.67165000	-1.01220200	-1.24419500
H	-5.74153800	-1.82138300	-0.10105900
C	-4.48527200	-0.33896400	0.78881000
H	-5.36831800	0.29668100	0.87289800
H	-4.30611300	-0.75752500	1.78444200
C	-3.74566300	1.90019700	-0.04959000
H	-4.66201400	1.79453600	-0.63535500
H	-3.96849900	2.53079800	0.81855700
C	-2.64191400	2.50452700	-0.90297000
H	-2.87227600	3.55368200	-1.10162200
H	-2.58530800	1.98185500	-1.86383300
C	-1.31168300	2.38519400	-0.17724300
H	-0.46776900	2.66271300	-0.80950600
H	-1.29561900	3.01732500	0.71789300

Sum of electronic and thermal Free Energies= -958.946125

Frequencies -- -349.5200 13.1995 25.2844

E'



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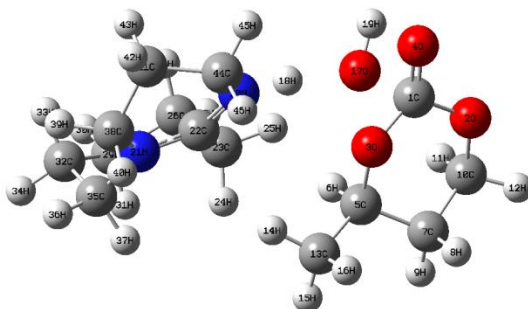
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O	2.36705400	0.75044400	0.36002400
O	3.27212000	1.30302300	-1.63404700
C	2.00675200	-0.27164600	1.29032200
H	1.22672300	-0.90459000	0.84219500
C	3.22090400	-1.14490700	1.57576400
H	3.98027000	-0.55650900	2.10686300
H	2.93807800	-1.99370100	2.20958600
C	3.77720600	-1.64293100	0.24939100
H	3.06855400	-2.34027900	-0.21933200
H	4.73284400	-2.15771400	0.38122300
C	1.43687400	0.41393700	2.51756700
H	0.56000100	1.01422800	2.25146600
H	1.13062300	-0.33162300	3.25912500
H	2.18441000	1.07296300	2.97347000
O	1.86029500	-0.51248200	-1.47843800
H	0.33611300	0.35509800	-1.03949200
H	2.03795500	-0.48206400	-2.42802900
N	-0.49146000	0.82180800	-0.64310100
N	-2.49285100	0.58593200	0.48993100

C	-1.44533800	0.06394400	-0.13745700
C	-1.33031600	-1.42187000	-0.33561900
H	-1.33354300	-1.92057600	0.64099300
H	-0.35565400	-1.61766200	-0.78846300
C	-2.44671000	-1.99092900	-1.23299400
H	-2.09011100	-2.94640800	-1.63109700
H	-2.58904500	-1.32610800	-2.09432500
C	-3.77803500	-2.22502100	-0.51607500
H	-4.48264400	-2.67839100	-1.22248300
H	-3.62134100	-2.96133500	0.28454600
C	-4.41732300	-0.97304900	0.08748200
H	-4.69526700	-0.26106700	-0.70014100
H	-5.34359000	-1.26099000	0.59723800
C	-3.52849500	-0.25716500	1.10547400
H	-4.12745800	0.41114100	1.72638100
H	-3.05547800	-0.97354900	1.78561600
C	-2.66477800	2.04188500	0.60907300
H	-3.73407300	2.25142900	0.52993500
H	-2.32878500	2.35278300	1.60510700
C	-1.90342200	2.77750200	-0.48298300
H	-1.92080700	3.84993300	-0.27587100
H	-2.39008700	2.61223700	-1.45021100
C	-0.47077000	2.27343300	-0.53680300
H	0.06063800	2.66252300	-1.40698800
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Sum of electronic and thermal Free Energies= -958.969966

Frequencies -- 22.2046 43.3679 45.0738

TS_{EF}'



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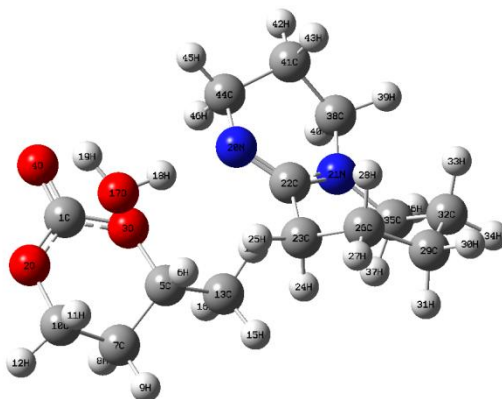
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O	2.41422800	0.71531300	0.48502200
O	3.38111300	1.48316800	-1.36636600
C	1.96962900	-0.41638800	1.25274000
H	1.18704300	-0.91707900	0.67349300
C	3.12743300	-1.38082700	1.43933800
H	3.90027900	-0.92536300	2.07070100
H	2.77796500	-2.29566700	1.92939300
C	3.68436700	-1.71279400	0.06761300
H	2.95199300	-2.27133000	-0.52391400
H	4.61582500	-2.27865000	0.12663800
C	1.38778700	0.13083000	2.53942500

H	0.57322300	0.83017900	2.32398100
H	0.98688600	-0.68931700	3.14387400
H	2.15363200	0.65340100	3.12291600
O	1.63499500	-0.44904100	-1.64729600
H	0.39193100	0.31448900	-1.12371800
H	1.86551500	-0.12608100	-2.52744100
N	-0.44425800	0.80674700	-0.65173700
N	-2.43800400	0.59956500	0.51641200
C	-1.41548900	0.07191100	-0.15917700
C	-1.36216900	-1.40944100	-0.41968500
H	-1.36023600	-1.94976500	0.53494900
H	-0.40565400	-1.61192200	-0.90802200
C	-2.51941500	-1.90117400	-1.31012700
H	-2.20858100	-2.85065900	-1.75844300
H	-2.65863200	-1.19475500	-2.13869800
C	-3.84246400	-2.12046500	-0.57285600
H	-4.57795400	-2.52040500	-1.28047700
H	-3.69336900	-2.89429600	0.19340700
C	-4.42414300	-0.87436800	0.09822700
H	-4.69326200	-0.12038400	-0.65268100
H	-5.34892100	-1.15195400	0.61683700
C	-3.48416100	-0.23426500	1.12143300
H	-4.04475200	0.42390700	1.78793900
H	-3.02111500	-0.99769500	1.75612900
C	-2.57286100	2.05323800	0.68128400
H	-3.63763400	2.29312500	0.62049800
H	-2.21919500	2.32934400	1.68192800
C	-1.80282500	2.80018500	-0.39689900
H	-1.78575200	3.86658000	-0.15897900
H	-2.30488100	2.67733300	-1.36292600
C	-0.38807500	2.24966300	-0.48264300
H	0.15280600	2.66345400	-1.33645200
H	0.18465000	2.48690500	0.42151900

Sum of electronic and thermal Free Energies= -958.961087

Frequencies -- -323.0129 28.0265 35.2414

F'



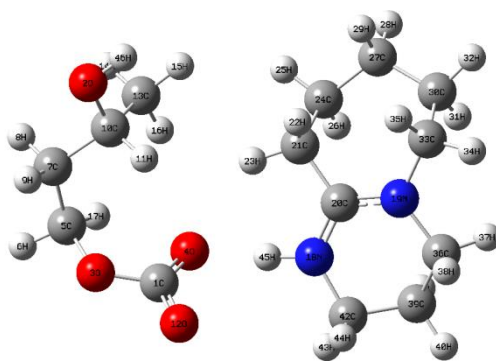
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O	-3.76423400	1.79485400	0.00099400
C	-1.67076000	-0.93165900	-0.87206700
H	-1.09349100	-1.05118400	0.04891300
C	-2.77856700	-1.96245600	-0.91824800
H	-3.33744400	-1.88383600	-1.85803500
H	-2.34969900	-2.96695300	-0.85603900
C	-3.68079100	-1.72484200	0.27051300
H	-3.15458500	-1.90118500	1.21206600
H	-4.59052100	-2.32401500	0.23716900
C	-0.75604000	-0.92517700	-2.07660800
H	-0.01303700	-0.12680500	-1.99034800
H	-0.22853200	-1.88258200	-2.13839600
H	-1.32695800	-0.78153800	-2.99973000
O	-1.74811100	0.05619100	2.36148200
H	-0.90788600	0.38897500	1.94287300
H	-2.21871200	0.84852500	2.64780400
N	0.51244900	0.97946500	1.04867000
N	2.15674700	0.57743600	-0.59606700
C	1.38652800	0.21559500	0.46847500
C	1.58170000	-1.17214500	1.03349400
H	1.35218200	-1.93059000	0.27255100
H	0.83828900	-1.28533300	1.82584200
C	2.99120900	-1.41714500	1.60394700
H	2.92308600	-2.23071700	2.33499500
H	3.31209900	-0.52528700	2.15901500
C	4.04658600	-1.79480500	0.56074900
H	4.99203400	-2.00951800	1.07317500
H	3.73665400	-2.73041700	0.07323600
C	4.29174900	-0.74072000	-0.51987200
H	4.71799400	0.17018900	-0.07884300
H	5.03193800	-1.12789700	-1.23082900
C	3.02850700	-0.36183300	-1.29745000
H	3.30160700	0.12230600	-2.23893400
H	2.46551200	-1.26264000	-1.57106600
C	2.19417600	1.96146500	-1.06883000
H	3.23801200	2.21925400	-1.28107500
H	1.63613100	2.04003000	-2.01245300
C	1.61639300	2.90436000	-0.02647800
H	1.45526700	3.89072000	-0.47175700
H	2.32468200	3.02141100	0.80264600
C	0.31333700	2.31371800	0.49889000
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Sum of electronic and thermal Free Energies= -958.990060

Frequencies -- 20.0545 35.1152 37.1026

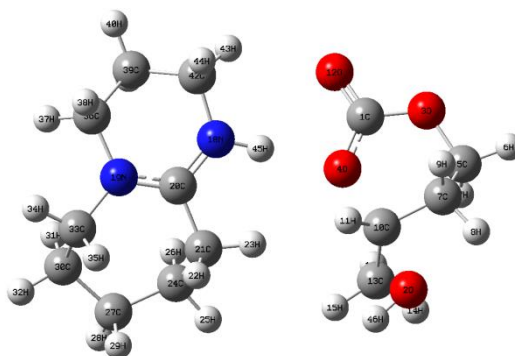
D S_N2



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O	-3.49587700	-1.71667100	0.07921900	
O	-1.48256300	-1.25864500	-0.85386600	
C	-4.11146800	-0.71484200	-0.73265100	
H	-5.05315300	-1.15301500	-1.07570600	
C	-4.40783000	0.54811000	0.06679800	
H	-5.08362600	1.18029600	-0.52520300	
H	-4.94603900	0.26559900	0.97954100	
C	-3.18520500	1.37187900	0.46047300	
H	-2.45206200	0.71932700	0.95558700	
O	-1.70536500	-2.80238000	0.76976500	
C	-2.52142100	2.06264000	-0.72433700	
H	-3.24253000	2.69925000	-1.24999300	
H	-1.68988100	2.69288200	-0.38698200	
H	-2.11984700	1.32489000	-1.42626800	
H	-3.48374900	-0.51001100	-1.60247000	
N	1.18283200	-1.38003500	-0.15922400	
N	3.00785700	-0.13383600	0.52602900	
C	1.73302600	-0.22605700	0.16059600	
C	0.87590700	1.00392900	0.05220000	
H	0.82360800	1.50077200	1.02842000	
H	-0.13575300	0.67044600	-0.18906700	
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H	0.53516000	2.62050700	-1.31059000	
H	1.66351300	1.42160000	-1.92118200	
C	2.53318000	2.88350600	-0.57159700	
H	2.77143300	3.58512600	-1.37899500	
H	2.19278700	3.49046200	0.27909800	
C	3.80830400	2.14205000	-0.16500600	
H	4.24252100	1.61846000	-1.02643900	
H	4.55109500	2.87481500	0.16986200	
C	3.59878100	1.13707300	0.96853400	
H	4.55464200	0.87889900	1.42788400	
H	2.97829500	1.56733200	1.76175300	
C	3.89870000	-1.30338000	0.50228100	
H	4.87997100	-0.95901000	0.16583500	
H	4.00493200	-1.68566200	1.52401000	
C	3.36987000	-2.37906600	-0.43372700	
H	3.95612300	-3.29167800	-0.30394600	
H	3.47630300	-2.05282100	-1.47390700	

C	1.90413500	-2.64405900	-0.12817800
H	1.45069300	-3.30471100	-0.86943100
H	1.78545700	-3.10797600	0.85759300
H	0.18025100	-1.38343600	-0.43628400
H	-2.90523500	2.87658100	1.69253000
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TS_{DE} S_N2



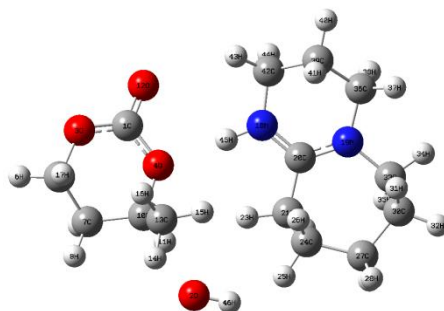
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O	3.79516800	1.59980100	-0.65105700
O	1.89352000	0.39059200	-0.40606100
C	4.52425500	0.37048300	-0.53789800
H	5.56396200	0.67696300	-0.42071400
C	4.07253100	-0.45656600	0.65189000
H	4.76817500	-1.28778200	0.78750300
H	4.10210000	0.15232100	1.56028200
C	2.70202800	-1.03885500	0.45113700
H	1.98208700	-0.94790300	1.24538600
O	1.82351900	2.57573600	-0.84343800
C	2.49514800	-2.08016200	-0.61850000
H	3.32966100	-2.78366800	-0.59812500
H	1.57349500	-2.64176700	-0.44985300
H	2.44329100	-1.61813000	-1.60796100
H	4.42776000	-0.18530300	-1.47706000
N	-0.83640100	1.10722600	0.28822600
N	-2.99420800	0.34581800	0.60757200
C	-1.71971600	0.12585200	0.31330200
C	-1.23743800	-1.25164400	-0.04223300
H	-1.40169400	-1.92454400	0.80771200
H	-0.15853200	-1.18614800	-0.18814800
C	-1.89521900	-1.81964900	-1.31355300
H	-1.23840200	-2.60972700	-1.69197600
H	-1.92372200	-1.03960800	-2.08467300
C	-3.29164300	-2.40555300	-1.09562300
H	-3.64311900	-2.84019600	-2.03803400
H	-3.21723300	-3.23385400	-0.37729300
C	-4.33506800	-1.40859400	-0.58779600
H	-4.51284700	-0.62256400	-1.33296300
H	-5.28645500	-1.93327600	-0.44572900

C	-3.96230400	-0.75345500	0.74259300
H	-4.84553500	-0.31473400	1.20993200
H	-3.57106800	-1.49426800	1.44795800
C	-3.51497800	1.70731600	0.80940600
H	-4.50990400	1.74353800	0.35891700
H	-3.62227500	1.88295300	1.88563500
C	-2.60900500	2.74639700	0.16773200
H	-2.92666200	3.74399100	0.47966400
H	-2.69296300	2.68958500	-0.92284600
C	-1.16807800	2.49572000	0.58227300
H	-0.46432100	3.11844500	0.02953300
H	-1.02987500	2.68170600	1.65331100
H	0.12410100	0.88244500	0.01015800
H	2.48501500	-3.22995800	1.98297300

Sum of electronic and thermal Free Energies= -958.921093

Frequencies -- -527.0069 20.4657 26.5635

E S_N2



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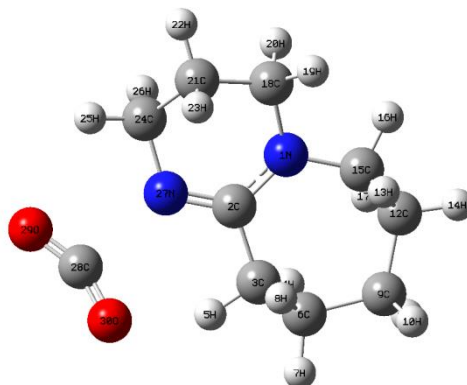
C	-2.85504400	1.34724000	-0.22508800
O	-1.21430900	-3.15176500	-1.65638800
O	-4.14875200	1.25696400	0.06021500
O	-2.08911000	0.25828800	-0.20939800
C	-4.76156600	0.01687600	0.49051300
H	-5.79615500	0.09142500	0.15696300
C	-4.04258900	-1.16864700	-0.10871000
H	-4.44895300	-2.09313900	0.31159100
H	-4.20126700	-1.19589200	-1.19203300
C	-2.55817300	-1.07964000	0.19097600
H	-1.99246000	-1.76106900	-0.46363000
O	-2.36593100	2.41871100	-0.52401600
C	-2.16895000	-1.30357100	1.64094300
H	-2.40410700	-2.33648900	1.91742700
H	-1.09233900	-1.15587700	1.76929500
H	-2.69052800	-0.63139800	2.33044300
H	-4.74267800	0.00878700	1.58326500
N	0.72344600	1.21345000	-0.37036300
N	2.96822800	0.67511000	-0.33157600
C	1.69563200	0.31960000	-0.44224100
C	1.31527800	-1.12168300	-0.61350600
H	1.78693300	-1.51219100	-1.52306900
H	0.23809500	-1.19052500	-0.78590800
C	1.70368100	-1.98946700	0.59843900

H	1.06764900	-2.88044100	0.57180300
H	1.45679600	-1.45451700	1.52468200
C	3.16995100	-2.42664400	0.61481200
H	3.33294300	-3.08704200	1.47390100
H	3.36681400	-3.02781700	-0.28372400
C	4.18320600	-1.28083000	0.66888300
H	4.09173100	-0.72803100	1.61265600
H	5.19403400	-1.70300700	0.64365600
C	4.06204200	-0.29572400	-0.49453400
H	4.97411500	0.29634300	-0.58641600
H	3.93588600	-0.82388200	-1.44518100
C	3.35761000	2.05940800	-0.01970700
H	4.22314200	2.01080600	0.64524000
H	3.66788600	2.55231200	-0.94775600
C	2.22005400	2.81180600	0.65181600
H	2.48027000	3.86991200	0.72757000
H	2.06686100	2.42640000	1.66546700
C	0.94610600	2.63915100	-0.15863500
H	0.07184700	3.03555000	0.35801200
H	1.02552000	3.14045000	-1.12945700
H	-0.23606100	0.87669100	-0.40959800
H	-0.27630200	-3.37210800	-1.73867900

Sum of electronic and thermal Free Energies= -958.950345

Frequencies -- 20.4548 32.1557 43.8578

[DBU-CO₂][‡]



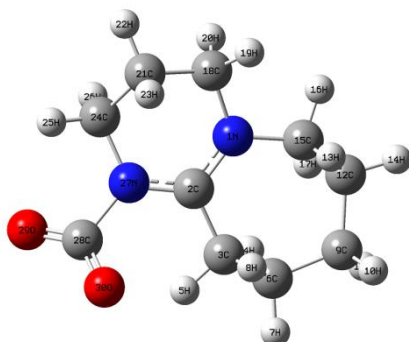
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C	0.00665200	0.03984100	-0.46914500
C	0.45772400	-1.37520300	-0.73546200
H	1.01558800	-1.41116200	-1.67983800
H	-0.43899200	-1.97472200	-0.87673000
C	1.30994100	-1.96900600	0.40150800
H	1.22680600	-3.06048100	0.34937500
H	0.87871900	-1.67000200	1.36596700
C	2.79314400	-1.59406300	0.34784500
H	3.31958300	-2.10313300	1.16424900
H	3.21818500	-1.98444200	-0.58811000
C	3.08270200	-0.09340400	0.42533300
H	2.78796100	0.30491200	1.40552900
H	4.16370900	0.06417700	0.32952000

C	2.37959900	0.72076800	-0.66489200
H	2.86151300	1.69634300	-0.77153300
H	2.47642700	0.22463600	-1.63685500
C	0.69442900	2.32583300	0.16513300
H	1.46714200	2.55133900	0.90893700
H	0.78139300	3.06878600	-0.63822000
C	-0.68495800	2.37953700	0.79732900
H	-0.97619300	3.42151200	0.95830600
H	-0.67620700	1.87734800	1.77179300
C	-1.66483100	1.66484000	-0.12532500
H	-2.67699400	1.67762700	0.28434800
H	-1.70253000	2.18087400	-1.09640100
N	-1.26713000	0.27872300	-0.32394300
C	-2.85197100	-1.08744500	0.08947600
O	-3.78536100	-0.39329800	-0.12998900
O	-2.31186000	-2.08818700	0.41995500

Sum of electronic and thermal Free Energies= -650.290099

Frequencies -- -226.9125 22.4771 35.5904

DBU-CO₂ Adduct



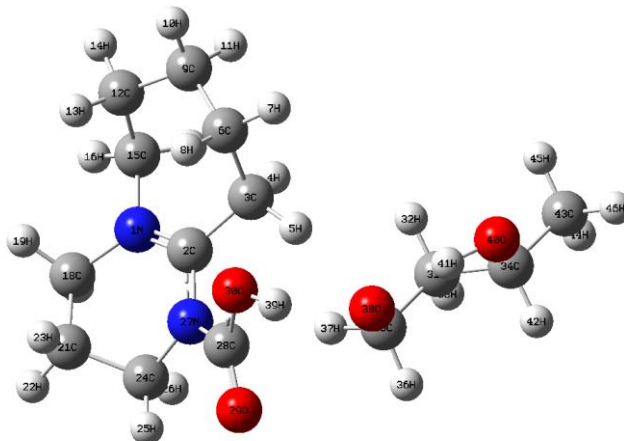
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N	0.73770600	1.02242300	-0.34784800
C	-0.05939000	-0.04454400	-0.36263100
C	0.55529900	-1.38196300	-0.67801000
H	1.07082900	-1.29529600	-1.64165500
H	-0.24010900	-2.10968700	-0.80389200
C	1.53708900	-1.86634600	0.40687000
H	1.59826100	-2.95691300	0.33197300
H	1.11982600	-1.64419200	1.39609000
C	2.94712800	-1.28723300	0.27508000
H	3.58210000	-1.70983700	1.06205500
H	3.37418000	-1.61830900	-0.68183500
C	3.02097600	0.23904200	0.34088000
H	2.72366600	0.59889200	1.33442900
H	4.06013400	0.55106800	0.18783100
C	2.16243200	0.94131600	-0.71256800
H	2.49212600	1.97395800	-0.84029400
H	2.26414700	0.46056700	-1.69003500
C	0.30798400	2.35224700	0.11278200
H	1.07193700	2.71791700	0.80496700
H	0.28860100	3.02120700	-0.75467500
C	-1.04620600	2.29157900	0.78794200
H	-1.45785500	3.29994200	0.87492200

H	-0.95498900	1.87385700	1.79608300
C	-1.96365000	1.41267400	-0.04255500
H	-2.94442300	1.30431700	0.41554300
H	-2.10299900	1.82740100	-1.04746500
N	-1.36914100	0.07542800	-0.14469700
C	-2.31518600	-1.08542300	0.03565800
O	-3.43043600	-0.88040300	-0.46466200
O	-1.87009400	-2.04559000	0.68004700

Sum of electronic and thermal Free Energies= -650.302910

Frequencies -- 51.9950 65.0546 89.1985

Proton Transfer [DBU-CO₂--primary OH][‡]

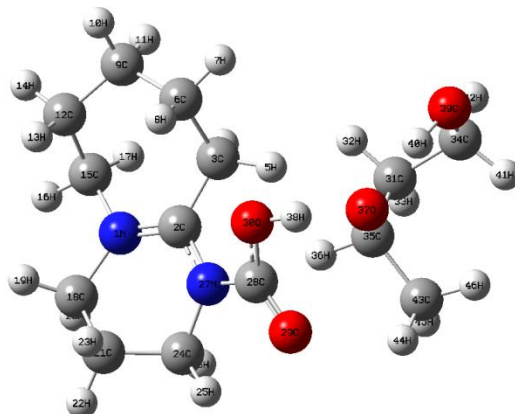


N	-1.23816900	-1.32038900	0.00660000
C	-0.49656300	-1.98467300	1.00614100
O	-0.19137400	-3.14928900	0.89856100
O	-0.34790300	-1.24606700	2.10167800
C	3.06582800	0.15284200	-1.26190700
H	2.54260200	1.10029100	-1.06122300
H	3.21622700	0.07911400	-2.34894200
C	4.42292700	0.19509400	-0.55651800
C	2.20086400	-1.02544800	-0.76863500
H	2.66623600	-1.96016600	-1.15766200
H	1.21900700	-0.95482800	-1.29447700
O	2.05243400	-1.05048000	0.60609600
H	0.42180100	-1.59423300	2.58031000
O	4.22848600	0.30130100	0.85101700
H	3.38244500	-0.23522400	0.99909200
H	4.94762000	-0.75367200	-0.77423800
C	5.30168900	1.34504700	-1.02408000
H	5.52567300	1.25090600	-2.09306700
H	4.79639200	2.30450100	-0.85823600
H	6.24963300	1.35533400	-0.47391600

Sum of electronic and thermal Free Energies= -958.932993

Frequencies -- -50.1705 19.3463 28.2971

Proton Transfer [DBU-CO₂--secondary OH][‡]



0 1

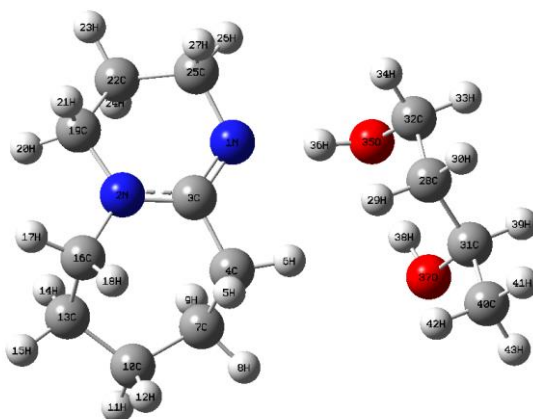
N	-2.34592000	0.10049400	-0.76458100
C	-1.23500700	-0.06042200	-0.08084900
C	-0.39074000	1.13161300	0.25604800
H	-0.21771900	1.66046800	-0.69076400
H	0.59276100	0.77787300	0.58766900
C	-1.03831600	2.09055100	1.27045100
H	-0.23242000	2.67592600	1.72508500
H	-1.49837600	1.51240000	2.07962000
C	-2.05825100	3.04615100	0.64922200
H	-2.46336400	3.70032400	1.42934700
H	-1.54080100	3.69769800	-0.06843800
C	-3.21766400	2.35339600	-0.06988500
H	-3.82171300	1.76993300	0.63671600
H	-3.87911500	3.11597100	-0.49504700
C	-2.78500600	1.43814900	-1.21772200

H	-3.62260000	1.25705900	-1.89202500
H	-1.98894100	1.89117700	-1.81542800
C	-3.29087500	-0.98153100	-1.10753300
H	-4.28089700	-0.65080500	-0.78292600
H	-3.29787300	-1.05850400	-2.19937700
C	-2.91438200	-2.30362200	-0.46980500
H	-3.39920700	-3.11766400	-1.01345500
H	-3.24674500	-2.34609000	0.57187300
C	-1.40542900	-2.44951900	-0.52349600
H	-1.05997300	-3.36974700	-0.05970700
H	-1.03155800	-2.41493800	-1.55174200
N	-0.82139100	-1.32501800	0.22451800
C	0.05011800	-1.64813100	1.28531500
O	0.60034800	-2.72210600	1.35013600
O	0.04003000	-0.72829900	2.24556700
C	3.03285800	0.88262600	-1.41952600
H	2.28128700	1.68086600	-1.33730600
H	3.21344800	0.71277000	-2.49071200
C	4.31949400	1.37012800	-0.75444000
C	2.46203000	-0.39588300	-0.75066500
H	1.46179500	-0.55588300	-1.22405300
O	2.33884400	-0.23815900	0.62088600
H	0.85764100	-0.83640500	2.75750500
O	4.10758300	1.62302800	0.62795100
H	3.41709700	0.92001500	0.86596600
H	5.11804900	0.62042700	-0.88465900
H	4.67206000	2.29722800	-1.22462900
C	3.29401000	-1.63676400	-1.11734300
H	2.83263100	-2.52792200	-0.67660600
H	3.36127300	-1.78255800	-2.20466900
H	4.31293900	-1.55411000	-0.71675600

Sum of electronic and thermal Free Energies= -958.931713

Frequencies -- -57.4820 30.1269 34.7379

Primary OH-DBU Adduct



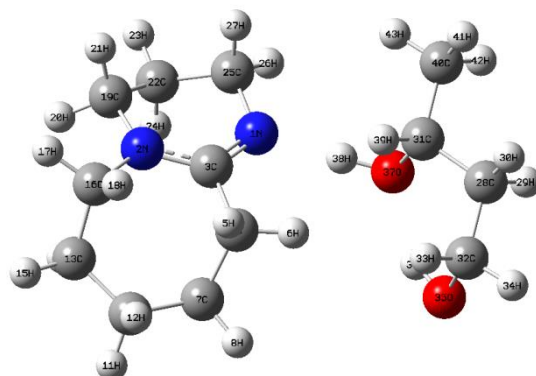
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C	-1.09960800	0.25820200	0.19803200
C	-0.38332000	-1.06752700	0.09645000

H	-0.37976500	-1.57396900	1.07062300
H	0.65797700	-0.84425800	-0.14164800
C	-0.96576000	-2.00395500	-0.97778500
H	-0.18184600	-2.71353600	-1.26621200
H	-1.20043400	-1.41675800	-1.87615300
C	-2.19614800	-2.79969900	-0.53463200
H	-2.49739500	-3.47242500	-1.34666400
H	-1.91051500	-3.44195800	0.31109900
C	-3.39790400	-1.95031000	-0.11608900
H	-3.78393300	-1.38200200	-0.97300200
H	-4.20366000	-2.61759600	0.21338400
C	-3.08649800	-0.97197000	1.02049000
H	-4.01492600	-0.64698000	1.49760400
H	-2.50093200	-1.47064700	1.80166800
C	-3.24277800	1.44070000	0.46890400
H	-4.21091400	1.13519400	0.05653200
H	-3.42498400	1.85854500	1.46810200
C	-2.58986000	2.47600200	-0.43254500
H	-3.11295400	3.43197000	-0.33516800
H	-2.66129000	2.15833100	-1.47974100
C	-1.12161400	2.60647700	-0.04469100
H	-0.60516000	3.31400600	-0.70150100
H	-1.04253300	3.00477000	0.97825900
C	3.23588300	0.58173500	0.86697800
H	2.31328300	0.16291800	1.29189900
H	3.86233400	0.90967100	1.70705200
C	3.97875000	-0.51347500	0.09790600
C	2.89797600	1.80345600	0.01165200
H	3.81902700	2.24808600	-0.38328000
H	2.39803000	2.56302700	0.62797600
O	2.08474600	1.47804900	-1.11120700
H	1.14331500	1.37088100	-0.77542500
O	3.18680800	-1.01551400	-0.98137600
H	2.71120200	-0.24368700	-1.34764200
H	4.90186600	-0.07535100	-0.31748500
C	4.35089300	-1.69179300	0.98220000
H	5.03284500	-1.37636500	1.77903400
H	3.45312400	-2.12349500	1.44019200
H	4.84713100	-2.47015900	0.39282200

Sum of electronic and thermal Free Energies= -770.467253

Frequencies -- 15.9050 20.6780 37.1053

Secondary OH-DBU Adduct

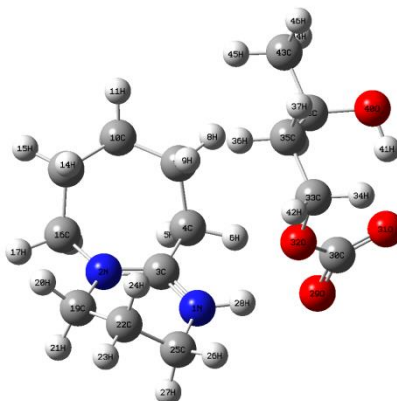


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N	-0.24430400	1.15064000	-0.29188200
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C	-1.08371900	0.26933300	0.16294100
C	-0.58030900	-1.14440100	0.34242100
H	-0.69255600	-1.45799800	1.38838700
H	0.49140300	-1.12106000	0.13471600
C	-1.26453700	-2.16502200	-0.58582700
H	-0.59074600	-3.02195400	-0.69864700
H	-1.37717400	-1.72181200	-1.58452900
C	-2.61682500	-2.67705400	-0.08238100
H	-2.98910700	-3.43967000	-0.77703300
H	-2.46191700	-3.18208900	0.88199600
C	-3.68813300	-1.60006900	0.09935500
H	-3.95242900	-1.15358700	-0.86861100
H	-4.59758500	-2.06884700	0.49428000
C	-3.26967800	-0.47950700	1.05604300
H	-4.15332000	0.06268800	1.40322200
H	-2.79854000	-0.90056400	1.95193800
C	-3.02318400	1.78315000	0.07085900
H	-4.00536500	1.55393200	-0.35758700
H	-3.18829900	2.39322500	0.96902800
C	-2.17160300	2.53497500	-0.93935800
H	-2.54344400	3.55847400	-1.04511500
H	-2.24067000	2.04939000	-1.92015200
C	-0.72143700	2.51419200	-0.47007400
H	-0.06782700	3.01479100	-1.19159600
H	-0.63085400	3.06420300	0.47896900
C	4.16960500	-0.26327300	0.51066300
H	4.90147500	0.07046700	-0.23774500
H	4.64910400	-0.18554100	1.49437100
C	2.95595900	0.66381900	0.48154300
C	3.80947900	-1.72504300	0.25416500
H	3.05266900	-2.04906900	0.98671600
H	4.68944600	-2.36239600	0.38455600
O	3.33197800	-1.94727000	-1.06836600
H	2.77604600	-1.16846500	-1.27021100
O	2.33765300	0.55600600	-0.80204000
H	1.36761400	0.79151200	-0.68117200
H	2.23765700	0.31381300	1.24099400
C	3.31547600	2.11440700	0.78079900

H	3.75750200	2.21198300	1.77921900
H	4.03585700	2.48732100	0.04313200
H	2.41922200	2.74322100	0.73770500
Sum of electronic and thermal Free Energies=			-770.466658
Frequencies --	15.4515	28.1864	32.5291

I



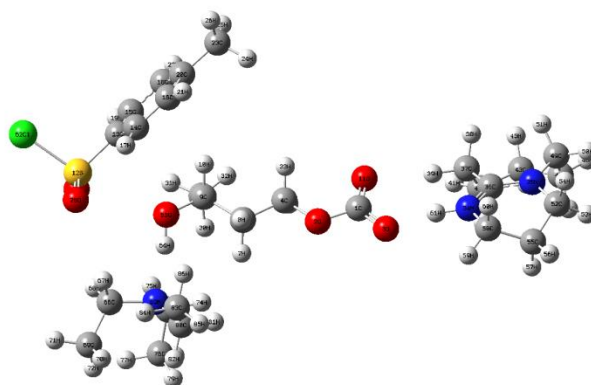
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N	-1.31388100	-1.59910200	-0.57465700
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C	-1.83684000	-0.39781600	-0.69086600
C	-1.12176200	0.59270100	-1.56727400
H	-1.79271600	0.92639400	-2.36791800
H	-0.29108100	0.06768200	-2.04427000
C	-0.59002800	1.80280700	-0.77514600
H	0.22328900	2.24622600	-1.35884000
H	-0.14201100	1.44704500	0.16105000
C	-1.62952000	2.88651900	-0.48565000
H	-1.13150900	3.72731600	0.01085200
H	-2.01306000	3.27234300	-1.44076400
C	-2.81324400	2.43277200	0.37076400
H	-2.47723300	2.15592600	1.37863800
H	-3.51033100	3.27062400	0.48626000
C	-3.58600400	1.25827600	-0.23166400
H	-4.57244100	1.17481500	0.22912300
H	-3.75493300	1.41267500	-1.30260400
C	-3.53155000	-0.92804600	0.98381700
H	-3.89614700	-0.29575700	1.79775400
H	-4.39377900	-1.44059200	0.54072200
C	-2.50956500	-1.92403700	1.50861000
H	-3.00995000	-2.65731500	2.14555700
H	-1.76033000	-1.40223200	2.11420100
C	-1.82548000	-2.61191300	0.33764400
H	-0.97453200	-3.21280300	0.66451700
H	-2.52351500	-3.26673600	-0.19623000
H	-0.38367500	-1.77639200	-1.01777500
O	1.14134500	-2.02040100	-1.67053600
C	2.05042600	-1.67424200	-0.87357400
O	3.26029400	-1.49856600	-1.11351600
O	1.57938500	-1.48170800	0.41545700
C	2.48332100	-1.03449700	1.42632500

H	3.49137400	-1.39429300	1.20525100
C	2.45673100	0.48121500	1.58720400
H	1.44378200	0.79058100	1.87864400
H	3.12799500	0.74509600	2.41605300
C	2.87998500	1.26675700	0.34077400
H	2.17034700	1.04530800	-0.47053400
O	4.18549900	0.90298100	-0.08488100
H	4.09738700	0.01549900	-0.48901700
H	2.14195900	-1.50968300	2.35033800
C	2.86521900	2.76556600	0.59483500
H	3.13339700	3.31002100	-0.31611700
H	1.87045300	3.09516100	0.91568300
H	3.58483900	3.02727600	1.37940300

Sum of electronic and thermal Free Energies= -959.009021

Frequencies -- 17.7697 33.7738 44.1567

II

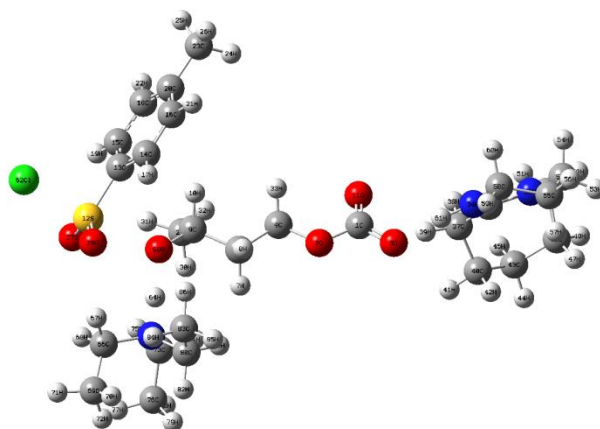


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O	1.37606943	-0.57908923	0.76858263
O	3.52286161	-0.62761434	1.23775406
C	0.32378992	-0.17828928	-0.10484213
H	0.48979987	-0.61063290	-1.09730134
C	-0.98245002	-0.66142908	0.50297006
H	-0.99275023	-1.76016712	0.51936626
H	-1.04147744	-0.32046137	1.54327655
C	-2.22498880	-0.15693722	-0.23763250
H	-2.22986122	0.93973229	-0.19695220
O	2.83561849	0.43342548	-0.63013929
S	-6.21363552	0.63242339	-0.01734033
C	-4.97190368	1.87429329	-0.20900699
C	-4.43346579	2.47390876	0.92558531
C	-4.56379722	2.21819642	-1.49196453
C	-3.44440966	3.43330690	0.75690314
H	-4.76306686	2.18147803	1.91627748
C	-3.57253230	3.18330863	-1.63585318
H	-4.99914693	1.73789011	-2.36194882
C	-2.99711762	3.79918170	-0.52003667
H	-3.00286981	3.89934813	1.63351651
H	-3.23699866	3.45185402	-2.63335857
C	-1.90552042	4.82506112	-0.67437016

H	-0.95827768	4.43858113	-0.28149834
H	-1.75298736	5.09155797	-1.72354873
H	-2.14364489	5.73705779	-0.11731245
O	-6.21808654	-0.27553191	-1.14513330
O	-6.27903585	0.15852433	1.34783919
C	-2.26486334	-0.58301787	-1.70427468
H	-2.13062661	-1.66705346	-1.80315646
H	-3.23172572	-0.31332896	-2.14017544
H	-1.47798215	-0.08894425	-2.28582562
H	0.32464687	0.91380280	-0.21096951
N	6.11407450	0.07264060	1.11405911
N	8.11759572	0.67029021	0.12463367
C	6.80096880	0.46753553	0.06332221
C	6.06185267	0.64696413	-1.23141780
H	6.19255170	1.67901905	-1.58015717
H	4.99329733	0.51849082	-1.02984162
C	6.52177991	-0.34106433	-2.32067303
H	5.71225227	-0.41818838	-3.05398341
H	6.63642954	-1.33930937	-1.87869316
C	7.80433060	0.06680848	-3.04975254
H	8.00924089	-0.66185332	-3.84248962
H	7.63109510	1.03047698	-3.54924736
C	9.04196726	0.19378356	-2.15879807
H	9.31202898	-0.78132860	-1.73264899
H	9.88953333	0.51883368	-2.77312363
C	8.87532747	1.19862346	-1.01734599
H	9.85083567	1.48808375	-0.62100189
H	8.39929928	2.11798097	-1.37482703
C	8.89308058	0.34276943	1.32910914
H	9.84421873	-0.08417993	0.99923469
H	9.10905395	1.27014273	1.87282757
C	8.15059121	-0.64990499	2.21009134
H	8.66614233	-0.74240118	3.16899917
H	8.14180218	-1.63603914	1.73331481
C	6.72157575	-0.17200945	2.41442726
H	6.11230727	-0.91888204	2.92687637
H	6.69895310	0.74991706	3.00719634
H	5.08973654	-0.13732142	1.02324993
Cl	-7.96522777	1.78620521	-0.26624692
N	-3.67467005	-3.32687486	0.82008234
H	-3.41738067	-1.54444179	0.53139211
O	-3.39928150	-0.55602418	0.44685559
C	-5.12477747	-3.29702400	1.05922797
H	-5.34928231	-2.39895732	1.64679598
H	-5.60138127	-3.14216770	0.08526732
C	-5.75542357	-4.50614489	1.75859317
H	-5.36569081	-4.63628055	2.77390547
H	-6.83600105	-4.34560132	1.84150039
H	-5.59285322	-5.44029741	1.21460444
C	-3.25996322	-3.97133095	-0.42690651
H	-2.19164880	-3.75221046	-0.55154018
H	-3.77959300	-3.45899188	-1.24597820
C	-3.47055890	-5.48317382	-0.56598370
H	-4.53092553	-5.73905565	-0.65013681
H	-2.97212311	-5.83730857	-1.47531536
H	-3.04843473	-6.03145542	0.28302248

C	-2.86634527	-3.71564627	1.97632616
H	-1.81838551	-3.69371770	1.65495936
H	-3.07291202	-4.75008187	2.29640278
C	-3.03763612	-2.77142857	3.16235999
H	-4.04488436	-2.82363268	3.58895240
H	-2.32893686	-3.04206333	3.95192937
H	-2.84729896	-1.73586183	2.86341728
Sum of electronic and thermal Free Energies=			-2530.641749
Frequencies --	8.1247	14.5563	16.3692

III

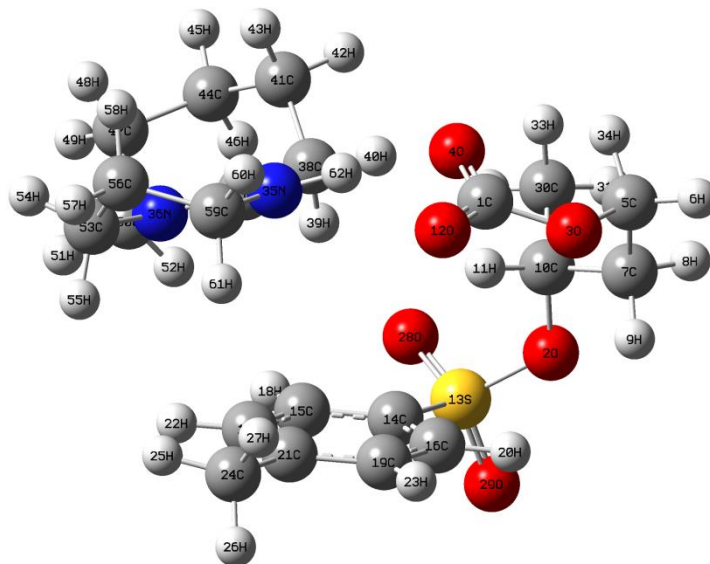


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C	0.51914308	0.06617434	-0.22557172
H	0.77454805	-0.17845607	-1.26194837
C	-0.80340923	-0.55699565	0.18948858
H	-0.75620580	-1.64017961	0.01305269
H	-0.94644728	-0.40631653	1.26631190
C	-2.01813421	0.04212993	-0.53727727
H	-1.95369701	1.13335614	-0.38470329
O	3.04742435	0.77244103	-0.51318988
S	-5.28443259	0.60123313	-0.10793750
C	-4.26279440	2.04566240	-0.15065639
C	-3.74530387	2.53530429	1.04053979
C	-4.00812230	2.64630825	-1.37587388
C	-2.93440892	3.66375209	0.98970880
H	-3.95539441	2.03828564	1.98111626
C	-3.19354273	3.77288538	-1.40046727
H	-4.43246476	2.24534580	-2.29037552
C	-2.64254976	4.29524826	-0.22501746
H	-2.51727331	4.05637189	1.91307365
H	-2.98390720	4.25204509	-2.35292900
C	-1.73341462	5.49592715	-0.27154093
H	-0.70298688	5.18765426	-0.48482633
H	-2.03826365	6.19447864	-1.05645113
H	-1.72916922	6.02926974	0.68333236
O	-5.47203787	-0.08467835	-1.37113340

O	-5.49028017	0.02494989	1.20551486
C	-1.97000780	-0.20308105	-2.05072033
H	-1.83072623	-1.26756210	-2.27598635
H	-2.90873275	0.12118231	-2.51016818
H	-1.14956815	0.35060823	-2.52368056
H	0.47420497	1.15930077	-0.14131211
N	6.14043093	0.49575106	1.05423294
N	8.16418681	0.63266013	-0.06047617
C	6.87703810	0.28792595	-0.01529649
C	6.23120515	-0.39967932	-1.18493311
H	6.31486064	0.24026404	-2.07151789
H	5.16480420	-0.48218799	-0.96702946
C	6.83903592	-1.78662320	-1.46673077
H	6.09959806	-2.35985184	-2.03534592
H	6.98176970	-2.31782363	-0.51690488
C	8.14719497	-1.75560074	-2.26136947
H	8.46518305	-2.78569096	-2.45917417
H	7.95218865	-1.29598173	-3.24046140
C	9.29678034	-1.00116324	-1.58884323
H	9.59659087	-1.50269399	-0.65940813
H	10.16734190	-1.01767003	-2.25481914
C	8.97131488	0.46064083	-1.27522474
H	9.89049493	1.02554126	-1.10727597
H	8.46359313	0.93656914	-2.12090024
C	8.85951409	1.15989754	1.12218013
H	9.86754612	0.73638638	1.12460503
H	8.95012332	2.24798989	1.02186840
C	8.13163432	0.78427611	2.40401363
H	8.57126576	1.32761967	3.24388078
H	8.24902856	-0.28771095	2.59635785
C	6.65438411	1.11715819	2.26533670
H	6.07303765	0.73403199	3.10614111
H	6.50085958	2.20135627	2.21232949
H	5.15001042	0.14216274	1.06246664
Cl	-7.19415275	1.83788367	-0.17312767
N	-3.57395614	-2.94305973	0.27950185
H	-3.39010479	-1.82353990	0.15935840
O	-3.20199002	-0.42192326	0.04539531
C	-5.05747162	-3.09103680	0.41390141
H	-5.39546553	-2.23515626	0.99968704
H	-5.46705157	-2.96516995	-0.59166110
C	-5.56064513	-4.38115360	1.05131522
H	-5.28938078	-4.45118671	2.10852860
H	-6.65358149	-4.37573587	0.99589591
H	-5.20550068	-5.28200956	0.54774051
C	-3.02037308	-3.52063618	-0.97844245
H	-1.95545459	-3.27233904	-0.97863623
H	-3.48341863	-2.95905146	-1.79492741
C	-3.20615923	-5.01525877	-1.19270066
H	-4.25016341	-5.27321023	-1.38672023
H	-2.62618634	-5.30824749	-2.07319623
H	-2.84442954	-5.60573245	-0.34563048
C	-2.81489381	-3.35315901	1.49316497
H	-1.75658088	-3.22822490	1.25165456
H	-2.98797607	-4.41560341	1.68471813
C	-3.16685542	-2.50179769	2.70480145

H	-4.19483326	-2.66127166	3.04273881
H	-2.49769471	-2.76783147	3.52832253
H	-3.03912100	-1.44075020	2.47456079
Sum of electronic and thermal Free Energies=			-2530.615106
Frequencies --	-214.1349	7.2967	13.5577

IV



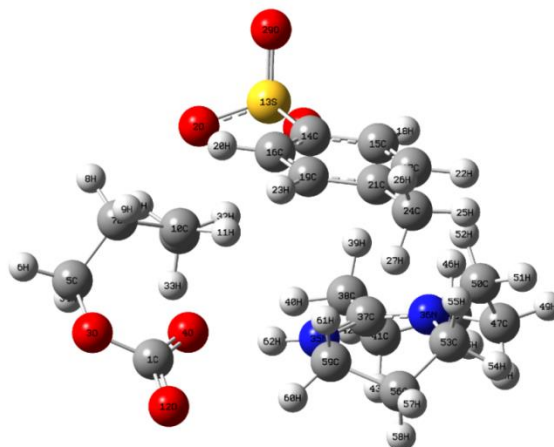
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O	-1.34386404	-2.29943540	0.02457863
C	-3.86751699	-1.44132632	0.16912249
H	-4.89437404	-1.70653378	0.43393349
C	-3.82539147	0.04196234	-0.19387897
H	-4.67840069	0.27235313	-0.84446758
H	-3.95619124	0.61804091	0.72814403
C	-2.54361370	0.49301953	-0.88737387
H	-1.67378483	0.13420807	-0.33012046
O	-1.19793755	-2.35468014	2.26918404
S	-1.19747692	2.76921387	-0.60297758
C	-0.53700323	2.09426542	0.89988679
C	0.81627995	1.78234705	0.96169701
C	-1.37303940	1.90253336	2.00013260
C	1.33354362	1.25740740	2.14186260
H	1.45859930	1.94912329	0.10365032
C	-0.84221012	1.36103097	3.16172030
H	-2.42691517	2.15634392	1.94590755
C	0.51502748	1.02279062	3.24877146
H	2.39305540	1.02389887	2.19635788
H	-1.49463114	1.18694211	4.01268204
C	1.06100762	0.39246644	4.50175139
H	2.15424550	0.35916613	4.49186888
H	0.74148774	0.94269282	5.39247237
H	0.68876890	-0.63390235	4.60097425
O	-0.26688060	2.45876986	-1.68196298

O	-1.61939785	4.14595878	-0.41492663
C	-2.45134116	0.07925083	-2.34306217
H	-3.32349863	0.43642830	-2.90033690
H	-1.54748179	0.47820298	-2.81046738
H	-2.41602390	-1.01301762	-2.40318939
H	-3.54349044	-2.07691059	-0.65838223
N	1.33831039	-1.83685703	0.35814137
N	3.08510065	-0.61839078	-0.54458985
C	1.83029213	-1.06434559	-0.58613867
C	0.93760717	-0.73293750	-1.74700314
H	0.80898498	0.35393327	-1.81682214
H	-0.04407406	-1.15279801	-1.52066176
C	1.45071467	-1.30119558	-3.08269986
H	0.59390490	-1.35171224	-3.76285824
H	1.78887846	-2.33437296	-2.93077657
C	2.55270627	-0.47314208	-3.74675080
H	2.80172570	-0.92639789	-4.71303531
H	2.15695522	0.52878078	-3.96373522
C	3.83383911	-0.32695122	-2.92256763
H	4.31600908	-1.30302845	-2.78076496
H	4.54200038	0.30041705	-3.47566895
C	3.60907564	0.31367811	-1.55229671
H	4.55028258	0.69201803	-1.14832735
H	2.93668038	1.17466634	-1.63655238
C	4.02754519	-1.07357851	0.48654293
H	4.99813885	-1.21543035	0.00305356
H	4.14284693	-0.28230184	1.23669601
C	3.56449265	-2.37361131	1.12777856
H	4.18194334	-2.58389521	2.00428090
H	3.68969767	-3.20058522	0.42046747
C	2.09976729	-2.26088287	1.52142269
H	1.69002343	-3.21461555	1.85574210
H	1.96014053	-1.53656626	2.33189781
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Sum of electronic and thermal Free Energies= -1777.716902

Frequencies -- 23.4218 29.4089 33.8111

V

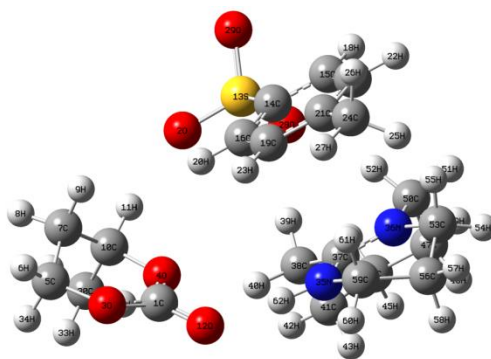


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O	-1.88020848	-2.18234315	-0.50559255
C	-4.36470733	-1.75120122	0.06318745
H	-5.35526874	-1.75224261	0.51926386
C	-3.75597561	-0.35194686	0.18977706
H	-4.51144191	0.37233485	-0.12937145
H	-3.52064147	-0.15424747	1.23824924
C	-2.55278192	-0.15907497	-0.67695881
H	-1.58100654	-0.05276890	-0.22421139
O	-1.71149707	-3.80383827	1.03825449
S	-1.37904014	2.74257203	-0.60307088
C	-0.30604935	2.19060859	0.72320738
C	1.06390953	2.41324017	0.61645656
C	-0.83059321	1.58192209	1.86151143
C	1.90834116	2.01801017	1.65008434
H	1.46767281	2.89478029	-0.26925851
C	0.02471337	1.18142270	2.88286080
H	-1.90039833	1.42361669	1.94949896
C	1.40496155	1.39500124	2.79588781
H	2.97669260	2.20072842	1.56121722
H	-0.38931640	0.69978922	3.76541487
C	2.31499745	0.95858676	3.91587819
H	3.36015944	1.20245995	3.70397372
H	2.03913440	1.44806078	4.85604866
H	2.24426344	-0.12276341	4.08382662
O	-0.65956757	2.41553754	-1.84944721
O	-1.63999536	4.17297367	-0.39127765
C	-2.68587541	-0.14725289	-2.16277463
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H	-2.61694733	-1.17403927	-2.53225493
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N	0.79953949	-1.74375108	0.24476636
N	2.78310189	-0.66566451	-0.24423746
C	1.53921941	-1.00624077	-0.56150472
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H	-0.07251365	-1.00636114	-1.90566116
C	1.71670131	-1.10839861	-3.10124727
H	1.02616627	-1.08070459	-3.95049303
H	1.97811415	-2.16304087	-2.94599296
C	2.96369450	-0.29998116	-3.46107668
H	3.38878228	-0.70284415	-4.38740286
H	2.66412314	0.73479170	-3.67748183
C	4.04701790	-0.28150070	-2.38206174
H	4.44766817	-1.28966203	-2.21507657
H	4.88124861	0.34056485	-2.72573437
C	3.55698679	0.28723329	-1.05110440
H	4.40238141	0.58690672	-0.42812710
H	2.95589644	1.18719008	-1.21673898
C	3.43994313	-1.18470150	0.96215781
H	4.48216836	-1.39052089	0.70302583
H	3.43200359	-0.40000875	1.72692135

C	2.76084429	-2.44791375	1.46794069
H	3.15835582	-2.70008436	2.45401197
H	2.97584768	-3.28328306	0.79302418
C	1.25807777	-2.22723051	1.54018018
H	0.71363934	-3.14787756	1.75422096
H	1.00257858	-1.48974582	2.30961939
H	-0.14241018	-2.01265176	-0.07414088
Sum of electronic and thermal Free Energies=			-1777.681407
Frequencies --	-432.3042	29.4527	33.5132

VI



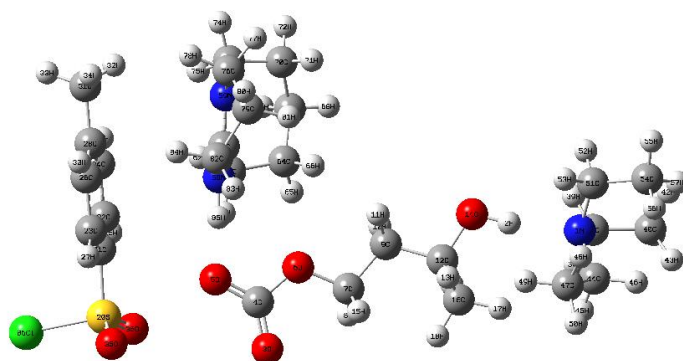
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O	-1.55389011	2.33757677	-1.30388870
O	-3.48974307	-2.39726191	0.96852931
O	-2.18515161	-1.39376606	-0.64091705
C	-4.64428037	-1.61201214	0.59005476
H	-5.23424609	-1.53228235	1.50240865
C	-4.21497150	-0.26359672	0.06008827
H	-5.08849669	0.28736507	-0.29965143
H	-3.75867837	0.32490579	0.86363681
C	-3.22499903	-0.45520519	-1.07512499
H	-2.66534565	0.46514119	-1.25532103
O	-1.39501394	-2.99485684	0.64288724
S	-0.23407158	2.94876451	-1.01719815
C	0.31074647	2.20769236	0.52904195
C	1.47713430	2.67167668	1.14040809
C	-0.40689713	1.16918437	1.10714261
C	1.90732232	2.09803229	2.32993624
H	2.04177967	3.48295206	0.68993771
C	0.03148487	0.60024449	2.30306308
H	-1.30555752	0.80769411	0.62108345
C	1.18890963	1.05625751	2.93419650
H	2.81323802	2.46812214	2.80522659
H	-0.54291613	-0.21050939	2.74567075
C	1.66672618	0.45467884	4.23194034
H	2.67726780	0.04020250	4.13019853
H	1.70818463	1.21176711	5.02271097
H	1.00429970	-0.34780054	4.56988258
O	0.80350779	2.56759453	-2.01011282
O	-0.29021315	4.40365092	-0.76429884
C	-3.81449406	-0.96623884	-2.37709302

H	-4.49896165	-0.21350085	-2.78036886
H	-3.01730076	-1.12914897	-3.10760086
H	-4.36314089	-1.90476626	-2.24822865
H	-5.20820044	-2.19084627	-0.14595114
N	1.26755845	-1.96129324	0.43210598
N	2.88606287	-0.43965133	-0.20115355
C	1.72846621	-1.04913917	-0.40966730
C	0.93962677	-0.77853195	-1.65514191
H	0.71767069	0.29204583	-1.72567734
H	-0.01497149	-1.29935821	-1.56757408
C	1.68566843	-1.23466289	-2.92568112
H	0.93410594	-1.37408062	-3.70981813
H	2.14353314	-2.21791382	-2.75366507
C	2.73040415	-0.23458066	-3.42875194
H	3.15605751	-0.61056445	-4.36646079
H	2.21974221	0.70763407	-3.66518144
C	3.86738556	0.06555832	-2.44849466
H	4.47893019	-0.83027889	-2.27394022
H	4.52664742	0.81804603	-2.89634890
C	3.37982098	0.61249816	-1.10622996
H	4.19459114	1.10432336	-0.57065818
H	2.59450742	1.35992734	-1.25487236
C	3.75495393	-0.79689959	0.92694726
H	4.78698785	-0.74295237	0.57051006
H	3.62879381	-0.04481752	1.71412449
C	3.45097540	-2.19604506	1.44097486
H	3.98684728	-2.36204519	2.37858629
H	3.79797383	-2.94047467	0.71627688
C	1.95390323	-2.35075633	1.65425408
H	1.68355890	-3.38514116	1.87437972
H	1.60965082	-1.72328527	2.48324472
H	0.33141178	-2.34204038	0.27739333

Sum of electronic and thermal Free Energies= -1777.729303

Frequencies -- 22.0009 27.7176 32.9174

VII



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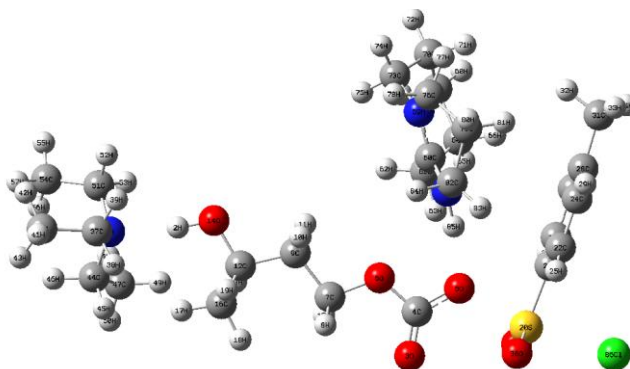
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C	-0.76295952	-2.17452520	0.42249914
O	-1.86623522	-1.58794870	0.61425754
O	0.27720002	-1.27692035	0.21675340
C	1.57878972	-1.82967594	0.05092143
H	1.58021192	-2.51148771	-0.80586122
C	2.54912153	-0.67538713	-0.14626215
H	2.39242528	-0.21489080	-1.12989517
H	2.34652418	0.09130038	0.61146511
C	4.01292814	-1.08747386	-0.02365880
H	4.15865984	-1.53225239	0.97547265
O	4.78209440	0.10100060	-0.12660911
H	1.84398867	-2.41504559	0.94083783
C	4.43812788	-2.11240999	-1.07237869
H	5.50515019	-2.34023470	-0.97243941
H	3.88891188	-3.05355611	-0.95847569
H	4.26151444	-1.72166104	-2.08155654
S	-4.75531175	-2.56000738	-0.19808379
C	-4.84918825	-0.81112753	0.05331013
C	-4.75110054	0.02969972	-1.05105827
C	-5.08441731	-0.32342608	1.33319657
C	-4.87745722	1.39786839	-0.85363932
H	-4.57200546	-0.37574594	-2.04141076
C	-5.20634658	1.05099820	1.50553942
H	-5.15914742	-0.99981593	2.17779482
C	-5.09962527	1.92912522	0.42268258
H	-4.79769901	2.06752923	-1.70616219
H	-5.38315151	1.44553156	2.50237600
C	-5.23187486	3.41669911	0.61406253
H	-4.49362434	3.95802171	0.01316837
H	-6.22396880	3.75965701	0.29818608
H	-5.10008748	3.69758442	1.66285336
O	-4.55341642	-3.25680868	1.05167894
O	-4.00971571	-2.86960850	-1.39793195
C	7.91364980	-0.30484417	-1.40234054
H	7.44425597	-1.19073170	-1.84729444
H	7.41242518	0.56434668	-1.84507051
C	9.39651908	-0.28204720	-1.78870806
H	9.49203798	-0.42706297	-2.87055337
H	9.86625123	0.67454949	-1.54160707
H	9.95822161	-1.08185377	-1.29430750
C	7.94330388	-1.56815747	0.69637985
H	7.64118544	-2.39017574	0.03703685
H	9.03386309	-1.65990704	0.82687029
C	7.25694039	-1.73681671	2.04781398
H	7.59874220	-0.99794264	2.77983210
H	6.17093969	-1.63824862	1.94913589
H	7.47545955	-2.72994437	2.45295537
C	7.90861998	0.90092953	0.76378296
H	7.72352481	1.73997944	0.08414290
H	7.18409429	1.00583200	1.58122053
C	9.31940620	1.01578971	1.35271522
H	9.42634851	1.99427916	1.83367585
H	9.50412639	0.25357546	2.11706059
H	10.09995682	0.92578618	0.59318181
N	-1.77897409	1.05601158	1.00220840

N	-1.60207526	3.17386164	0.08897182
C	-1.64932689	1.84614307	-0.03794800
C	-1.48261958	1.20584787	-1.38701312
H	-2.25694423	1.56908055	-2.07174348
H	-1.64265332	0.13378228	-1.25927821
C	-0.08554248	1.46871918	-1.97966517
H	0.11558567	0.67907404	-2.71090716
H	0.66467042	1.35527016	-1.18886940
C	0.06251276	2.82750613	-2.66869087
H	1.06062402	2.89080903	-3.11684442
H	-0.65599907	2.88131538	-3.49901393
C	-0.15016834	4.04119534	-1.76024723
H	0.62908453	4.08540201	-0.98824847
H	-0.05684734	4.95443161	-2.35919458
C	-1.51868129	4.06174190	-1.07660076
H	-1.74664131	5.06395914	-0.70687360
H	-2.31094812	3.80448743	-1.78779857
C	-1.52352710	3.81097931	1.41022959
H	-0.83730938	4.65808613	1.32468819
H	-2.51221251	4.20354926	1.67651856
C	-1.02094282	2.83314845	2.46124879
H	-1.12455218	3.28083319	3.45259374
H	0.04052307	2.62087876	2.29323598
C	-1.82029054	1.54278028	2.37106350
H	-1.40543423	0.76236544	3.01234728
H	-2.86160449	1.70843481	2.67025114
H	-1.78284977	0.01618123	0.83742690
Cl	-6.76746623	-2.96735554	-0.71051864

Sum of electronic and thermal Free Energies= -2530.640391

Frequencies -- 9.4236 14.6462 19.7709

VIII



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N	-7.42656735	-0.18446820	-0.03122072
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O	0.64254133	-3.52296537	-0.16879781
C	0.84235548	-2.33004047	-0.01245281
O	1.98162090	-1.70862734	0.07055642
O	-0.16593971	-1.42743850	0.10130218
C	-1.50113447	-1.93975620	0.04474155
H	-1.62595909	-2.68994949	0.83117394

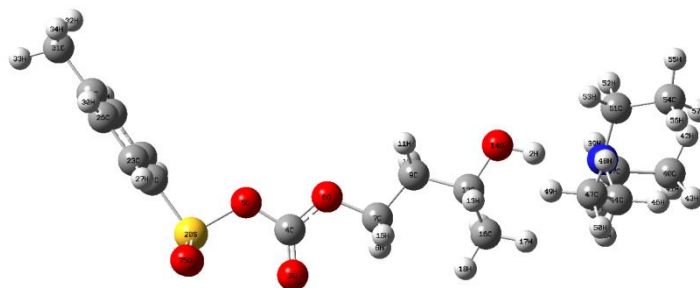
C	-2.43227890	-0.75427904	0.22732803
H	-2.29434892	-0.32447988	1.22785681
H	-2.16635010	0.01967440	-0.50228472
C	-3.90575103	-1.10317022	0.03290258
H	-4.02684738	-1.52688786	-0.97856554
O	-4.62268578	0.11736915	0.12273341
H	-1.65920683	-2.42909798	-0.92298274
C	-4.41951445	-2.12292252	1.04662037
H	-5.48986099	-2.30084961	0.89853640
H	-3.91098448	-3.08734387	0.93998515
H	-4.26837193	-1.75579013	2.06861012
S	3.77943360	-2.75294098	-0.04667340
C	4.41805624	-1.09641302	0.11244751
C	4.70356702	-0.60886115	1.37815914
C	4.58207534	-0.33563681	-1.03680538
C	5.14910197	0.70486325	1.49144860
H	4.58535696	-1.23745369	2.25470892
C	5.04153230	0.96792049	-0.89716796
H	4.36423311	-0.75147870	-2.01467834
C	5.31016874	1.51487020	0.36343606
H	5.37177177	1.10341558	2.47774668
H	5.19107414	1.57206933	-1.78802662
C	5.73703450	2.95382366	0.49264535
H	4.87710428	3.62161298	0.35520691
H	6.16578694	3.15757204	1.47784495
H	6.47878121	3.21809859	-0.26736058
O	3.51929771	-3.20322120	-1.39353329
O	3.53131849	-3.45794200	1.18890116
C	-7.76615205	-0.16762130	1.39523266
H	-7.32439365	-1.07155504	1.83212690
H	-7.23757655	0.68159689	1.84480823
C	-9.24713393	-0.10233333	1.78328115
H	-9.34609108	-0.25454372	2.86379838
H	-9.68761498	0.87043519	1.54582674
H	-9.83376638	-0.87963130	1.28213027
C	-7.84717816	-1.40742855	-0.71607381
H	-7.58550502	-2.24729791	-0.06196535
H	-8.93974405	-1.45061090	-0.85266236
C	-7.16049434	-1.59455222	-2.06483242
H	-7.46349505	-0.83401147	-2.79162044
H	-6.07162808	-1.54676492	-1.95870024
H	-7.42160981	-2.57266328	-2.48105110
C	-7.72022342	1.05865098	-0.75918895
H	-7.50541042	1.88372125	-0.07133527
H	-6.99327991	1.14612323	-1.57658353
C	-9.12656497	1.22805796	-1.34528812
H	-9.19969466	2.21376486	-1.81762938
H	-9.33911984	0.47961775	-2.11583451
H	-9.90881222	1.15906839	-0.58536842
N	1.65074859	0.90521703	1.07178149
N	0.89566334	3.04417019	0.64295456
C	1.19817681	1.81524273	0.23375507
C	1.07150510	1.43572303	-1.21441976
H	0.01823570	1.50821738	-1.51191326
H	1.34611785	0.38288642	-1.30129644
C	1.95554958	2.29009323	-2.14180603

H	2.11109409	1.71827972	-3.06244846
H	2.94212962	2.41153165	-1.68034950
C	1.37776690	3.65889583	-2.50324097
H	2.04277436	4.14084118	-3.22878266
H	0.41292785	3.51655858	-3.00972991
C	1.17516926	4.59679694	-1.31247933
H	2.13865990	4.84711477	-0.84958328
H	0.73795687	5.53639074	-1.66900458
C	0.24721672	4.02296931	-0.24246250
H	-0.11731735	4.81752220	0.41165961
H	-0.63624182	3.56394733	-0.69899942
C	1.16898597	3.49329081	2.01649241
H	1.55067497	4.51623713	1.95315142
H	0.22297147	3.51796986	2.56966602
C	2.18335541	2.59391355	2.70548972
H	2.22014960	2.83643519	3.77002234
H	3.18082839	2.76068436	2.28408204
C	1.78829825	1.14089413	2.50001359
H	2.54659292	0.45575468	2.88107639
H	0.83972861	0.91510370	3.00132446
H	1.82999242	-0.03831798	0.70450428
Cl	6.14088773	-3.48448515	-0.12843091

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Frequencies -- -243.2391 6.1101 10.5185

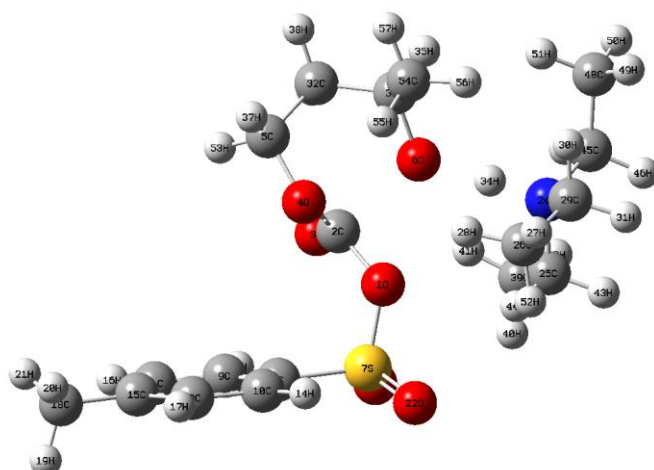
IX



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C	-1.78802500	-1.33335600	0.08853800
O	-2.94929000	-0.61549400	0.06146400
O	-0.80132700	-0.46346100	0.02684500
C	0.53520300	-1.02184500	0.06190600
H	0.59775500	-1.79953000	-0.70237600
C	1.49834400	0.12070900	-0.19106600
H	1.38218900	0.48160300	-1.21999900
H	1.25539500	0.95072200	0.48138700
C	2.95878800	-0.26960200	0.03638100
H	3.07590700	-0.56096800	1.09405300
O	3.72037200	0.89604300	-0.22121500
H	0.68581600	-1.47867000	1.04527600
C	3.41078700	-1.43758000	-0.83743100
H	4.47585600	-1.63704700	-0.68039400

H	2.86945900	-2.35830100	-0.59238400
H	3.25439700	-1.20874000	-1.89808600
S	-4.41133100	-1.44319500	0.04026800
C	-5.43847800	-0.01216500	-0.00024300
C	-5.72004500	0.58335600	-1.22909000
C	-5.93501300	0.49990300	1.19534900
C	-6.51909700	1.71845200	-1.24887800
H	-5.32294000	0.16680500	-2.14887300
C	-6.73580200	1.63570100	1.15027200
H	-5.70542900	0.01965200	2.14047800
C	-7.03851100	2.25942100	-0.06507000
H	-6.74346700	2.19302600	-2.20004800
H	-7.13094900	2.04249200	2.07674100
C	-7.92641500	3.47483000	-0.10857300
H	-7.57222500	4.19699100	-0.85029800
H	-8.94757200	3.18989200	-0.38794400
H	-7.97303800	3.97082300	0.86464900
O	-4.54997300	-2.13341300	1.30471200
O	-4.48013700	-2.15978200	-1.21577800
C	6.81854800	0.21494000	-1.46987100
H	6.35229200	-0.75348700	-1.68687700
H	6.29533900	0.95336600	-2.08927900
C	8.29209100	0.15903800	-1.88571400
H	8.36692300	-0.24410700	-2.90180400
H	8.75220400	1.15155600	-1.89071800
H	8.87731600	-0.49026900	-1.22572700
C	6.89046400	-0.53746800	0.86143000
H	6.57556700	-1.48669500	0.41247000
H	7.98316900	-0.60204900	0.98949800
C	6.22690400	-0.39038100	2.22709900
H	6.58255200	0.49327800	2.76662100
H	5.13938800	-0.30990900	2.12598800
H	6.45133500	-1.26713200	2.84303400
C	6.86896300	1.88186700	0.36165700
H	6.67861900	2.54418300	-0.48981800
H	6.16273900	2.18409500	1.14513900
C	8.29296900	2.10796200	0.88288500
H	8.42824000	3.17368400	1.09733100
H	8.47789800	1.56139400	1.81359600
H	9.05676000	1.80987200	0.16040500
Sum of electronic and thermal Free Energies=			-1608.065006
Frequencies --	7.9408	16.9451	22.1324

X



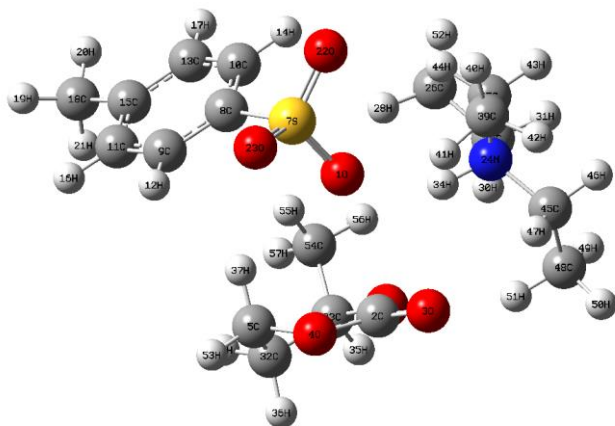
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C		-0.18005378	0.73019248	-0.64972091
O		-0.41596008	0.72699978	-1.83685860
O		-0.53573442	1.68429504	0.22551894
C		-0.39574846	3.03217219	-0.26481325
O		1.81506873	1.05514566	-0.49093233
S		-1.14065569	-1.68238646	-0.14002628
C		-2.71649967	-0.90531666	0.06078563
C		-3.40384943	-0.45637044	-1.06410304
C		-3.22280500	-0.72383327	1.34613129
C		-4.62589417	0.18267000	-0.88889873
H		-2.98453760	-0.59940939	-2.05383067
C		-4.44664373	-0.08381528	1.49845319
H		-2.67089700	-1.07883172	2.21033922
C		-5.16551535	0.37577389	0.38783835
H		-5.16776644	0.53796036	-1.76113891
H		-4.85109453	0.06001296	2.49667701
C		-6.50739916	1.03774009	0.56123745
H		-7.30872972	0.29161656	0.50307347
H		-6.58583209	1.53275943	1.53344469
H		-6.68892008	1.77970418	-0.22187070
O		-0.86549521	-2.55850342	0.98654613
O		-1.01743652	-2.20204250	-1.48780487
N		3.38797902	-0.81181275	0.24072371
C		2.72859870	-2.06703272	-0.23057143
C		2.28744378	-0.93086812	2.50291453
H		2.50046159	-0.71640872	3.55448298
H		1.55792019	-0.20150049	2.14076561
C		3.58719305	-0.82627405	1.71739674
H		4.08105760	0.11078879	1.97576435
H		4.27531093	-1.64517119	1.95914462
C		0.98756843	3.27715752	-0.86595131
C		2.08091407	2.40453023	-0.22343943
H		2.69364321	0.04907150	-0.01970999
H		3.02757264	2.69279419	-0.71707175
H		0.97311434	3.05802423	-1.93754973
H		-0.56318341	3.63851603	0.62712420
H		1.23104528	4.34000078	-0.74907337
C		2.40019330	-2.05912594	-1.71627202

H	1.73486807	-2.90048274	-1.92743309
H	1.87134160	-1.14086242	-1.98770483
H	3.28738653	-2.16756241	-2.34629863
H	3.38370952	-2.90561424	0.03477176
H	1.80563686	-2.16465046	0.33830123
C	4.66191267	-0.57492541	-0.49910885
H	5.27549821	-1.47938506	-0.41225533
H	4.38543711	-0.45085408	-1.54683485
C	5.43781762	0.65338259	-0.04518933
H	5.92364950	0.51596426	0.92412870
H	6.22175377	0.85363102	-0.78132566
H	4.79437588	1.53704515	0.00251510
H	1.83666256	-1.92469614	2.45032378
H	-1.19399302	3.23682401	-0.98531204
C	2.24438940	2.68722183	1.27593947
H	1.35162220	2.38268128	1.83118160
H	3.09589649	2.12721976	1.67914459
H	2.42947172	3.75309020	1.46089179

Sum of electronic and thermal Free Energies= -1608.035018

Frequencies -- -307.4046 19.9832 27.4765

XI



O	1		
O	0.42945818	-0.47712740	-0.82662690
C	1.87771206	1.64042374	-1.85835137
O	2.80218992	0.96660356	-2.26179269
O	0.87570399	1.96734028	-2.66687915
C	-0.32267344	2.53362871	-2.10823149
O	1.89534171	2.09990368	-0.60524634
S	-0.73823823	-1.38314883	-1.04995121
C	-2.06653746	-0.62446127	-0.11155349
C	-2.94116165	0.26743496	-0.72847847
C	-2.16846821	-0.86812965	1.25556220
C	-3.89540437	0.93578658	0.03355038
H	-2.88400901	0.42648287	-1.80093884
C	-3.12699117	-0.19465025	2.00803919
H	-1.50896776	-1.58974531	1.72765169
C	-3.99651367	0.72526609	1.41334238

H	-4.57711849	1.62881568	-0.45420293
H	-3.20109187	-0.39189699	3.07473656
C	-5.01389662	1.47931674	2.23218695
H	-5.97753418	1.53154988	1.71521255
H	-5.17240061	1.00707332	3.20600341
H	-4.68101478	2.50888869	2.40958332
O	-0.52549785	-2.71863774	-0.45107306
O	-1.17823412	-1.40105991	-2.45746575
N	2.98809286	-1.11852047	0.29789814
C	2.66221868	-2.56766098	0.06009667
C	1.45654981	-1.07285779	2.31520329
H	1.37586568	-0.59612350	3.29659957
H	0.66351426	-0.68123712	1.67459558
C	2.82066044	-0.73472822	1.73916613
H	2.97912983	0.34312221	1.78334187
H	3.62808860	-1.22613445	2.29045151
C	0.04820242	3.61993500	-1.12612425
C	0.91651304	3.01750441	-0.03130809
H	2.27797706	-0.59436976	-0.24461299
H	1.53463801	3.79324070	0.42722426
H	0.58497937	4.41827672	-1.64909943
H	-0.88536629	1.72521940	-1.63692365
H	-0.85377572	4.05186457	-0.68288482
C	2.82761425	-2.98128530	-1.39271966
H	2.37707478	-3.96988785	-1.51455650
H	2.29553494	-2.29132805	-2.05521479
H	3.87283751	-3.04677650	-1.70561368
H	3.30404055	-3.14692143	0.73094727
H	1.61860177	-2.69986712	0.34350992
C	4.36450295	-0.78524940	-0.21326213
H	5.02256658	-1.58015407	0.15039574
H	4.30246276	-0.84497017	-1.29828803
C	4.88796966	0.58148965	0.19491894
H	5.15428282	0.63298064	1.25397314
H	5.79707040	0.77048331	-0.38355141
H	4.17065243	1.36922940	-0.04483253
H	1.30740340	-2.14652187	2.45090528
H	-0.88129324	2.91195304	-2.96356811
C	0.14579221	2.27610118	1.04689021
H	-0.46751413	1.47573026	0.62584251
H	0.83786192	1.83336034	1.76932426
H	-0.50052509	2.98188287	1.57902183
Sum of electronic and thermal Free Energies=			-1608.110886
Frequencies --	22.2510	24.8830	32.4676

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